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RESEARCH REPORT No. CX-42

Relativistic Coulomb Scattering

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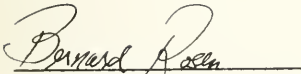
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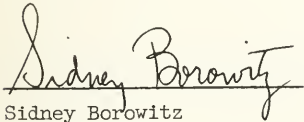
Research Report No. CX - 42

RELATIVISTIC COULOMB SCATTERING

Bernard Rosen

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Bernard Rosen

A handwritten signature in cursive script, reading "Sidney Borowitz", written over a horizontal line.

Sidney Borowitz
Acting Project Director

April, 1959

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Abstract

Contour integration is employed to evaluate analytically the correction terms to the Rutherford cross section for high energies. The sum of partial waves is replaced by an equivalent integral which is expanded in powers of the fine structure constant. Evaluation of the resultant integrals is performed wherever possible by use of integral representations for the transcendental functions appearing in the integrands; an unsuccessful attempt to determine the values of the integrals by the saddle point approximation is briefly sketched. Those terms which appear in the cross section to the fifth order in the fine structure constant are explicitly given by closed analytic expressions.

The general form of the correction term corresponding to an arbitrary power of the fine structure constant is found in terms of two dimensional integrals involving elementary transcendental functions.

A related problem, the non-relativistic scattering for an attractive $1/r^2$ potential, is also discussed.

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1. Introduction

In recent years several investigations, [1], [2]* both theoretical and experimental, have been undertaken to determine the structure of nuclei (including the proton) from the results of the scattering of fast (i.e., relativistic) electrons by nuclei. The experimental data and the theoretical results measure essentially the deviation of the actual scattering from that due to a point nucleus and thus reveal certain details of the charge distribution. It is this scattering by a point charge that will concern us in this paper.

Since the structure to be investigated has dimensions of the order of 10^{-13} cm it is necessary to use short wavelength, i.e., high speed, electrons with the velocity (v) of the electrons close to the speed of light (c). Thus, in order to determine the scattering, one must use the appropriate solution of Dirac's relativistic wave equation.

The appropriate solutions of the wave equation in terms of a partial wave expansion for scattering of fermions by a static Coulomb potential were first derived by Mott [3] and have been well known for many years. The corresponding phase shifts are of a complicated enough form, however, that the summation of the partial waves in the relativistic case, in contrast to those obtained by solution of the non-relativistic Schrödinger equation, cannot be readily accomplished. Two approaches have to be used to determine the differential cross section for different energies and nuclear charges - the first, essentially a numerical calculation, and the second, an expansion of the wave function (or phase shift) in powers

*

Both of these review articles contain references to a rather extensive literature.

of the two parameters Z (the nuclear charge) times the fine structure constant (e^2/hc)^[4] and the ratio $\beta = v/c$.

Bartlett and Watson^[5] were the first to carry out a calculation of the first sort, and their work has been extended recently by Yadav^[6], Doggett and Spencer^[7] and Sherman^[8]. Yadav gives results for uranium at energies of 0.145, 0.314, 0.666, 3.350 and 20.000 Mev; Sherman gives extensive tables for $Z = 13, 48$ and 80 , for $\beta = 0.2, 0.4, 0.5, 0.6, 0.8$ and 0.9 and for angles between 15° and 165° in fifteen degree intervals. Doggett and Spencer, whose work was approximately simultaneous with that of the last two sources, published results for $Z = 6, 13, 29, 50, 82$ and 92 , at energies ranging from moderate (0.05 Mev) to relativistic (10 Mev) over the entire angular range. They estimated that their error was less than 0.5% except at the largest angles.

Mott^[3],^[9] carried out an expansion of the phase shift to determine the lowest-order deviation of the differential cross section from the Rutherford cross section $\sigma_R(\theta)$ where:

$$(A) \quad \sigma_R(\theta) = \frac{(Ze^2)^2}{4m^2v^4} (1-\beta^2) \csc^4 \theta/2$$

where m is the mass of the scattered particle, v its velocity, and θ the angle of scattering. He found the ratio R between the differential cross section and $\sigma_R(\theta)$ to be

$$(B) \quad R \equiv \frac{\sigma(\theta)}{\sigma_R(\theta)} = 1 - \beta^2 \sin^2 \theta/2 + \pi\beta \sin \theta/2 \cos^2 \theta/2 + \dots$$

Following this, Sexl^[10] using the second Born approximation, found instead

$$R = 1 - \beta^2 \sin^2 \theta/2 + \pi\beta \sin \theta/2 + \dots ;$$

and this result was verified by the work of Urban^[11] who used an expansion of the phase shift. Dalitz^[12] and Schwinger^[13] however, found that

$$(C) \quad R = 1 - \beta^2 \sin^2 \theta / 2 - \pi \alpha \beta \sin \theta / 2 (1 - \sin \theta / 2)$$

and this result has been confirmed by the recent work of McKinley and Feshbach^[14] and Feshbach^[15] and Curr^[16]. McKinley and Feshbach carried out an expansion of the phase shifts to the fourth order in $\alpha \equiv Z \times e^2 / hc$. In their paper some of the resulting series of the form

$$\sum_{0 \text{ or } 1}^{\infty} f(n) P_n(\cos \theta)$$

where evaluated in closed form and the remainder evaluated numerically. The most extensive calculation of this sort has been carried out by Curr who expanded the phase shift to order α^8 and calculated the angle-dependent coefficients numerically. By comparison with the work of Yadav he estimates that his error is of the order of $\frac{1}{9} (\alpha/\beta)^9$ for energies greater than 0.5 Mev.

In this paper we shall first present an outline of the Mott calculation and then present a calculation along the lines indicated by McKinley and Feshbach, and Curr. This calculation will, however, employ a technique borrowed from electromagnetic field calculations, which is often denoted by the generic term, the Watson transformation^[17]. By use of this last method it is possible to evaluate in closed form all the angular coefficients of the powers of α that enter into the differential cross section to order α^5 in terms of elementary transcendental functions and the dilogarithm of Euler. We then show how

the coefficient of an arbitrary power of α can be expressed in terms of sums of two-dimensional integrals whose integrands contain only elementary transcendental functions. Inasmuch as certain of the sums of Legendre functions times functions of angular momentum quantum number contained in the papers alluded to above converge very poorly, equivalent integrals may be more amenable to calculations. Finally, we indicate the nature of the functions required to express the angular dependence of the higher order correction terms to the cross-section.

2. Formulation of the problem

2.1 The Mott formula^[18]

According to Dirac, the wave equation obeyed by electrons in a force field with a scalar potential V (vector potential $\vec{A} = 0$) is given by

$$(1) \quad \left\{ \left[E - eV/c \right] + \vec{\alpha} \cdot \vec{p} + \beta mc \right\} \psi = 0$$

where ψ is the four component spinor

$$(2a) \quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} .$$

In (1) p is the momentum, m the mass, and E the energy of the particle; $\vec{\alpha}$ and β are the 4×4 matrices indicated symbolically by

$$(2b) \quad \alpha_1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

Here σ_1 are the usual 2×2 Pauli spin matrices and 1 is the 2×2 unit matrix.

Before considering the Coulomb case proper, one first develops the formalism for potentials which decrease at infinity at least as rapidly as $\frac{1}{r^{\epsilon+1}}$, $\epsilon > 0$. Consider those solutions with $E > mc^2$ that obey the following boundary conditions:

$$(3a) \quad \psi_\lambda \text{ finite at the origin}$$

and

$$(3b) \quad \psi_\lambda \xrightarrow{r \rightarrow \infty} a_\lambda e^{ikz} + \frac{e^{ikr}}{r} u_\lambda(\theta, \phi)$$

where r, θ, ϕ are the usual spherical coordinates and k is the momentum divided by \hbar . The differential cross section is given by

$$(4) \quad \sigma(\theta, \phi) = \sum_1^4 |u_\lambda(\theta, \phi)|^2 / \sum_1^4 |a_\lambda|^2 .$$

Since it can be shown that

$$(5) \quad \left| \frac{a_2}{a_4} \right| = \left| \frac{a_1}{a_3} \right| \quad \text{and} \quad \left| \frac{u_2}{u_4} \right| = \left| \frac{u_1}{u_3} \right| ,$$

the cross section simplifies to

$$(6) \quad \sigma(\theta, \phi) = \frac{|u_3|^2 + |u_4|^2}{|a_3|^2 + |a_4|^2} .$$

If the beam is considered to be polarized along the direction of propagation (z), then the solution desired is of the form

$$(7a) \quad \psi_3 \xrightarrow{r \rightarrow \infty} e^{ikz} + f(\theta, \phi) e^{ikr}/r$$

$$(7b) \quad \psi_4 \xrightarrow{r \rightarrow \infty} g(\theta, \phi) e^{ikr}/r$$

where r , θ , and ϕ are the usual spherical coordinates.

By expanding the wave function in spherical harmonics Darwin [19] found the following pairs of solutions for the partial waves:

$$(8a) \quad (\psi_3)_n = (n+1)P_n(\cos\theta)G_n(r), \quad (\psi_4)_n = -G_n(r)P_n^{(1)}(\cos\theta)e^{i\phi};$$

$$(8b) \quad (\psi_3)_{-n-1} = nP_n(\cos\theta)G_{-n-1}(r), \quad (\psi_4)_{-n-1} = G_{-n-1}P_n^{(1)}(\cos\theta)e^{i\phi}$$

where G_n is a solution of the coupled equations

$$(9a) \quad \frac{1}{\hbar} \left(\frac{E}{c} - \frac{eV}{c} + mc \right) F_n + \frac{dG_n}{dr} - \frac{n}{r} G_n = 0,$$

$$(9b) \quad \frac{1}{\hbar} \left(\frac{E}{c} - \frac{eV}{c} - mc \right) G_n + \frac{dF_n}{dr} + \frac{n+2}{r} F_n = 0,$$

after the F_n are eliminated. F_n represents the radial wave functions associated with ψ_1 and ψ_2 . G_{-n-1} satisfies the equation corresponding to (9a,9b) with n replaced by $-n-1$. If the asymptotic form of the G 's is taken to be ($r \rightarrow \infty$),

$$(10a) \quad G_n \sim \frac{1}{r} \sin(kr - \frac{n\pi}{2} + \eta_n)$$

$$(10b) \quad G_{-n-1} \sim \frac{1}{r} \sin(kr - \frac{n\pi}{2} + \eta_{-n-1})$$

then $i^n e^{i\eta_n} G_n$ and $i^n e^{i\eta_{-n-1}} G_{-n-1}$ are the radial functions that will have the desired asymptotic form. Finally, then, the wave functions

are given by

$$(11a) \quad \psi_3 = \sum_{n=0}^{\infty} \left\{ (n+1) e^{i\eta_n} G_n + n e^{i\eta_{-n-1}} G_{-n-1} \right\} i^n P_n(\cos \theta)$$

$$(11b) \quad \psi_4 = \sum_{n=0}^{\infty} \left\{ -e^{i\eta_n} G_n + e^{i\eta_{-n-1}} G_{-n-1} \right\} i^n P_n^{(1)}(\cos \theta) e^{i\phi}$$

or

$$(12a) \quad \left\{ \begin{aligned} 2ikf(\theta, \phi) &= \sum_{n=0}^{\infty} \left\{ (n+1) (e^{2i\eta_n} - 1) + n (e^{2i\eta_{-n-1}} - 1) \right\} P_n(\cos \theta) \end{aligned} \right.$$

$$(12b) \quad \left\{ \begin{aligned} 2ikg(\theta, \phi) &= \sum_{n=1}^{\infty} (-e^{2i\eta_n} + e^{2i\eta_{-n-1}}) P_n^{(1)}(\cos \theta) e^{i\phi} \end{aligned} \right.$$

For the case of the Coulomb interaction, as in the non-relativistic formalism, we keep (11a) and (11b), but the phase shift is determined by comparison of the asymptotic form of the G's with

$$\frac{1}{r} \sin(kr + \gamma \ln 2kr - \frac{n\pi}{2} + \eta_n)$$

where $\gamma \equiv Ze^2/hv \equiv \alpha \frac{c}{v} \equiv \alpha/\beta$.

Mott [3] solves (9) to find

$$(13a) \quad e^{2i\eta_{-n-1}} = \frac{n-i\gamma'}{\rho_n^{-i\gamma}} \frac{\Gamma(\rho_n+1-i\gamma)}{\Gamma(\rho_n+1+i\gamma)} e^{i\pi(n-\rho_n)}$$

$$(13b) \quad e^{2i\eta_n} = -\frac{n+1+i\gamma'}{\rho_{n+1}^{-i\gamma}} \frac{\Gamma(\rho_{n+1}+1-i\gamma)}{\Gamma(\rho_{n+1}+1+i\gamma)} e^{i\pi(n-\rho_{n+1})}$$

with $\rho_n = +\sqrt{n^2 - \alpha^2}$, $\gamma' = \gamma \sqrt{1 - \beta^2}$, and $\Gamma(x)$ is the usual Gamma function.

Using the abbreviations

$$(14a) \quad C_n = -e^{-i\pi\rho_n} \Gamma(\rho_n - i\gamma) / \Gamma(\rho_n + 1 + i\gamma)$$

$$(14b) \quad F(\theta) = \frac{1}{2} \sum (-1)^n \left\{ n C_n + (n+1) C_{n+1} \right\} P_n(\cos \theta)$$

$$(14c) \quad G(\theta) = \frac{1}{2} \sum (-1)^n \left\{ n^2 C_n - (n+1)^2 C_{n+1} \right\} P_n(\cos \theta),$$

Mott finds that [20]

$$(15a) \quad k f(\theta) = -i\gamma' F + G$$

$$(15b) \quad k g(\theta) = \left\{ i\gamma' (1 + \cos \theta) F + (1 - \cos \theta) G \right\} / \sin \theta$$

where he has used the relations [23]

$$(16a) \quad P_{n+1}(\cos \theta) = \cos \theta P_n + \frac{\sin \theta}{n+1} P_n^{(1)}(\cos \theta)$$

$$(16b) \quad P_{n-1}(\cos \theta) = \cos \theta P_n - \frac{\sin \theta}{n} P_n^{(1)}(\cos \theta).$$

Expanding F and G in powers of α , Mott gets

$$(17a) \quad F = F_0 + \alpha F_1 + \dots$$

$$(17b) \quad G = G_0 + \alpha G_1 + \dots$$

and, corresponding to the lowest approximation,

$$(18a) \quad \sigma(\theta) = \frac{(Ze^2)^2}{4m^2 v^2} \csc^4\left(\frac{\theta}{2}\right) \left(1 - \frac{v^2}{c^2}\right) \left(1 - \frac{v^2}{c^2} \sin^2 \theta/2\right)$$

and

$$(18b) \quad \sigma(\theta) = \frac{(Ze^2)^2}{4m^2 v^2} \csc^4\left(\frac{\theta}{2}\right) \left(1 - \frac{v^2}{c^2}\right) \left(1 - \frac{v^2}{c^2} \sin^2 \theta/2 + \pi \alpha \frac{v}{c} \sin \frac{\theta}{2}\right)$$

corresponding to the next higher approximation.

2.2 The method of contour integration [22], [23], [24], [25]

If we have a series of the form

$$(19) \quad S = \sum_{n=0}^{\infty} f(n) P_n(\cos \theta)$$

the Cauchy integral theorem allows us to write the sum as either

$$(20a) \quad S = \frac{1}{2} \int_C \frac{f(v) P_v(\cos \theta) dv}{e^{+i\pi v} \sin \pi v}$$

or

$$(20b) \quad S = \frac{1}{2} \int_C \frac{f(v) P_v(-\cos \theta) dv}{\sin \pi v}$$

where C is the path indicated in Figure 1 in a complex v plane whose

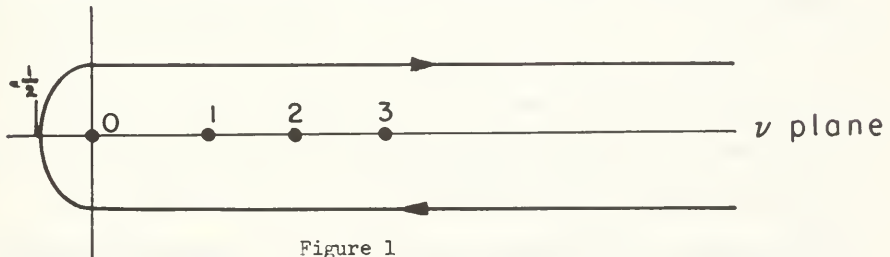


Figure 1

real axis coincides at the integers with the values of the orbital angular momentum quantum numbers. By the use of this integral we assume that $f(v)$ possesses the proper analytic behavior so that Cauchy's theorem holds. One also has the choice, of course, of replacing $f(v)$ in the integral by any function $\phi(v)$ such that $\phi(n) = f(n)$, for all integers n , provided the integral is still defined. It may

then be possible, by properly distorting or otherwise modifying the path C , to evaluate the integral by one of the following methods:

- a) Saddle point approximation
- b) Sum of residues of the function $f(v)$
- c) Explicit evaluation by use of integral representation for $f(v)$ and P_v .

The first two methods are most often used in the study of electromagnetic wave propagation at short wavelength; the second representation is the result of the so called Watson transformation proper. We shall actually find that the third method is the most useful for evaluating the relativistic correction terms.

The most often encountered application of these analytic techniques has been in the study of the propagation of waves in spherically or cylindrically stratified media. Specific calculations have been made in such topics as diffraction and reflection by conducting and dielectric spheres^[26], diffraction by smooth objects^[27], and radio propagation^[24]. These methods are most useful in problems in which the wavelength is small compared to the scatterer of the radiation, i.e., where k (the wave number or $2\pi/\text{wavelength}$) times a (the size of the scatterer) is much greater than unity. Under these circumstances the sum of partial waves will contain such a larger number (of the order of ka) of significant terms that a numerical evaluation would ordinarily be called for; the use of this technique allows one to determine the behavior of the scattered field in an asymptotic expansion involving powers (often fractional) of $(\frac{1}{ka})$. In the mathematical theory of optics these ideas have proved invaluable in treating the transition from wave to geometrical optics^[28].

In this paper we shall apply the method of contour integration (or, alternatively, the Watson transformation) to obtain, insofar as possible, closed expressions for the angular dependence of the relativistic Coulomb differential cross section. Before proceeding with a detailed discussion of the relativistic case we shall apply this method to the well-known non-relativistic scattering problem. Here it is known that the sum of partial waves obtained by solving Schrödinger's equation for a particle in a Coulomb field is exactly summable in terms of a single confluent hypergeometric function. We shall see that the method of contour integration, while unnecessary in this instance, is capable of giving the correct answer approximately without great analytic difficulty. What 'approximately' means will be discussed shortly.

The Schrödinger equation^[29] will have the form

$$(21) \quad -\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{Ze^2}{r} \psi = E\psi, \quad E > 0$$

with the boundary conditions

ψ regular at the origin

$$(22) \quad \psi \xrightarrow{r \rightarrow \infty} e^{ikz - i\gamma \ln k(r-z)} + \frac{e^{ikr + i\gamma \ln 2kr}}{r} f(\theta).$$

The solution required is, if v again denotes the velocity of the particle,

$$(23) \quad \psi = \frac{1}{v^{1/2}} \Gamma(1-i\gamma) e^{\pi\gamma/2} e^{ikz} \Phi(1\gamma, 1, ik\xi),$$

$$\xi = r(1 - \cos \theta) = 2r \sin^2 \theta/2.$$

in parabolic coordinates, and is

$$(24) \quad \psi = \frac{1}{\sqrt{1/2}} e^{\pi\gamma/2} \sum_{n=0}^{\infty} \frac{\Gamma(n+1-i\gamma)}{(2n)!} (2ikr)^n e^{ikr} \Phi(n+1-i\gamma, 2n+2, -2ikr) P_n(\cos \theta)$$

in spherical coordinates. Here Φ is the confluent hypergeometric function of the first kind. The solutions here are normalized to unit incident flux. By the method of contour integration one should be able to get from (24) to (23).

Using the relations [30]

$$(25) \quad \Phi(a, c, x) = e^x \Phi(c-a, c, -x) \quad \text{[Kummer's transformation]}$$

and [31]

$$(26) \quad \Phi(a, c, x) = \frac{\Gamma(c)}{\Gamma(c-a)} e^x x^{\frac{1}{2} - \frac{1}{2}c} \int_0^{\infty} e^{-t} t^{-\frac{1}{2}c-a-\frac{1}{2}} J_{c-1} [2(xt)^{1/2}] dt$$

$$\operatorname{Re} c > \operatorname{Re} a > 0, \quad \operatorname{Re} x > 0$$

in succession, one obtains [32]:

$$(27) \quad \psi = \frac{1}{\sqrt{v}} e^{ikr} e^{\pi\gamma/2} \sum_{n=0}^{\infty} \int_0^{\infty} \frac{e^{-t} t^{-i\gamma}}{u} (2n+1) P_n(\cos \theta) J_{2n+1}(2u) dt$$

where $u = \sqrt{2ikrt}$. No difficulties arise from the violation of the condition $\operatorname{Re} x > 0$ in (26). Indeed the same equation is used again in reverse to obtain the final answer. One can consider that

$$(28) \quad 2ikr = \lim_{\epsilon \rightarrow 0} \epsilon + 2ikr.$$

Actually one need go no further to prove the equivalence of the two relations (23) and (24). As a special case of a theorem due to Bailey [33] one has

$$(29) \quad u J_0(2u \sin \frac{\theta}{2}) = \sum (2n+1) J_{2n+1}(2u) P_n(\cos \theta);$$

using (26) with $c = 1$, $a = i\gamma$, we get

$$(30) \quad \psi = \frac{1}{\sqrt{v}} \exp [\pi\gamma/2 + ikz] \quad \Gamma(1-i\gamma) \Phi(1\gamma, 1, 2ikr \sin^2 \theta/2).$$

A theorem due to Erdélyi^[27] could have been used to circumvent the intermediate steps.

It should be interesting to see if we can get this result approximately by means of a saddle point evaluation. Furthermore the discussion will serve as a guide when we consider the more complex relativistic scattering. Again, by means of the Cauchy integral theorem

$$(31) \quad \begin{aligned} F(u, \theta) &= \sum_{n=0}^{\infty} (2n+1) J_{2n+1}(2u) P_n(\cos \theta) \\ &= \frac{1}{2} \int \frac{(2v+1) J_{2v+1}(2u) P_v(\cos \theta)}{\sin \pi v e^{+i\pi v}} dv \end{aligned}$$

where C is the path of integration shown in Figure 1.

The result of a saddle point evaluation, by virtue of the assumptions made in the method, holds, strictly, only asymptotically; that is, if $f_s(u, \theta)$ is the result of a saddle point approximation for the function $f(u, \theta)$, $f(u, \theta) - f_s(u, \theta) \xrightarrow{u \rightarrow \infty} 0$. In other words, the first term in the asymptotic expansion of the integral in (31) (as obtained by the method of steepest descent) should be equal to the first term in the asymptotic expansion (large u) of $u J_0(u \sin \theta/2)$.

We shall assume first that a saddle point lies in the first quadrants and that $\text{Im } v_{sp} \gg 0$, where v_{sp} denotes the position of this point.

Then [34]

$$(32a) \quad e^{i\pi\nu} \sin \pi\nu \xrightarrow{\text{Im}\nu \rightarrow \infty} -\frac{1}{2i}$$

$$(32b) \quad P_\nu(\cos \theta) \xrightarrow{\text{Im}\nu \rightarrow \infty} \frac{\Gamma(\nu+1)}{\Gamma(\nu+\frac{3}{2})} \sqrt{\frac{2}{\pi \sin \theta}} \cos \left[\left(\nu + \frac{1}{2} \right) \theta - \frac{\pi}{4} \right]$$

$$(32c) \quad \frac{\Gamma(\nu+1)}{\Gamma(\nu+\frac{3}{2})} = \frac{\Gamma(\nu+\frac{1}{2}+\frac{1}{2})}{\Gamma(\nu+\frac{1}{2}+1)} \xrightarrow{\text{Im}\nu \rightarrow \infty} (\nu + \frac{1}{2})^{-1/2}$$

and [35]

$$(32d) \quad J_{2\nu+1}(2u) \rightarrow \frac{e^{2i u \sin \chi - i(2\nu+1)\chi}}{2\sqrt{\pi i u \sin \chi}}, \quad \cos \chi = \frac{2\nu+1}{2u}.$$

Using these relations in (31),

$$(33) \quad F(u, \theta) = \int_{c'} \frac{u}{\sqrt{\pi^2 i \sin \theta}} \sqrt{\cos \chi \sin \chi} (e^{iR_+} + e^{iR_-}) d\chi$$

where

$$\begin{aligned} R_{\pm} &= 2u \sin \chi - (2\nu+1) \chi \pm \left(\nu + \frac{1}{2} \right) \theta \mp \frac{\pi}{4} \\ &= 2u \left[\sin \chi - \chi \cos \chi \pm \frac{\theta}{2} \cos \chi \right] \mp \frac{\pi}{4}. \end{aligned}$$

The position of the saddle point in the first quadrant is given by the solution of

$$(34) \quad \frac{\partial R_+}{\partial \chi} = 0$$

and is $\chi_{sp} = \theta/2$, $v_{sp} + \frac{1}{2} = u \cos \frac{\theta}{2}$. The equation of the fall line or path of steepest descent, is given by

$$(35a) \quad \text{Im} \left[2i u \sin \chi + i(2v+1) \chi + i(v + \frac{1}{2})\theta - \frac{i\pi}{4} \right] = \text{Im} \left[2i u \sin \chi_{sp} + \frac{i\pi}{4} \right]$$

or

$$(35b) \quad \text{Re} \left[u \sin \chi - (v + \frac{1}{2}) \left(\chi - \frac{\theta}{2} \right) \right] = \sqrt{krt \sin^2 \theta/2}.$$

In the neighborhood of v_{sp} we place $(\chi = \chi_s + ds e^{i\phi})$ and obtain

$$\text{Re} \left[+ \frac{ds^2 e^{2i\phi}}{\sqrt{2}} e^{i\pi/4} \right] = 0.$$

The solution $\phi = \pi/8$ yields an exponent which decreases as one moves away from the saddle points. The results for R_- are obtained in a similar fashion.

The contribution to $f(u, \theta)$ from the saddle point evaluation is given by

$$(36) \quad f_{sp} = u \frac{\cos(2u \sin \frac{\theta}{2} - \frac{\pi}{4})}{\sqrt{\pi u \sin \theta/2}}.$$

Since

$$(37) \quad J_o(2u \sin \theta/2) \xrightarrow{u \rightarrow \infty} \frac{1}{\sqrt{\pi u \sin \theta/2}} \cos(2u \sin \theta/2 - \pi/4) + O\left(\frac{1}{u^{3/2}}\right)$$

we have $f(u, \theta) - f_{sp}(u, \theta) \xrightarrow{u \rightarrow \infty} 0$. We shall employ the method of steepest descents in order to estimate the relativistic correction terms in the next section, but, unfortunately, the results are not useful.

2.3 Relativistic wave function and method of steepest descent

Here we consider not the phase shifts but the wave functions themselves. Mott finds for the G's :

$$(38a) \quad G_{-n-1} = \frac{1}{2} \frac{e^{-ikr} e^{\pi\gamma/2}}{r \Gamma(2\rho_n+1)} (2kr)^{\rho_n} \frac{|\Gamma(\rho_n+1+i\gamma)|}{\sqrt{\rho_n-i\gamma} (-i\sqrt{n-i\gamma'})} \\ \times \left\{ (\rho_n-i\gamma) \phi(\rho_n+i\gamma, 2\rho_n+1, 2ikr) - (n-i\gamma') \phi(\rho_n+1+i\gamma, 2\rho_n+1, 2ikr) \right\}$$

and

$$(38b) \quad G_n = \frac{1}{2} \frac{e^{-ikr} e^{\pi\gamma/2}}{r \Gamma(2\sigma_n+1)} (2kr)^{\sigma_n} \frac{|\Gamma(\sigma_n+1+i\gamma)|}{\sqrt{\sigma_n-i\gamma} \sqrt{n+1+i\gamma'}} \\ \times \left\{ (\sigma_n-i\gamma) \phi(\sigma_n+i\gamma, 2\sigma_n+1, 2ikr) + (n+1+i\gamma') \phi(\sigma_n+1+i\gamma, 2\sigma_n+1, 2ikr) \right\}$$

where $\sigma_n = \rho_{n+1}$.

It is convenient to deviate from the procedure of previous authors by splitting off the term that in the limit $c \rightarrow \infty$ yields the non-relativistic wave function. For this purpose we use the identities [37]

$$(39a) \quad \phi(\rho_n+i\gamma, 2\rho_n+1, 2ikr) = \phi(\rho_n+1+i\gamma, 2\rho_n+1, 2ikr) - \frac{2ikr}{2\rho_n+1} \phi(\rho_n+1+i\gamma, 2\rho_n+2, 2ikr)$$

and

$$(39b) \quad \phi(\sigma_n+i\gamma, 2\sigma_n+1, 2ikr) = \frac{\sigma_n+i\gamma}{-\sigma_n+i\gamma} \phi(\sigma_n+1+i\gamma, 2\sigma_n+1, 2ikr) \\ + \frac{2\sigma_n}{-\sigma_n+i\gamma} \phi(\sigma_n+i\gamma, 2\sigma_n, 2ikr).$$

In addition to this we use an integral representation for the ϕ 's mentioned previously in this paper. One finds that:

$$(40a) \quad e^{i\eta_{-n-1}G_{-n-1}} = \left\{ \rho_n^{-n+i(\gamma'-\gamma)} \right\} \frac{1}{2} \exp \left[\frac{i\pi\eta}{2} - i\pi\rho_n + ikr + \frac{\pi\gamma}{2} \right] \int_0^\infty e^{-t} t^{-i\gamma-1} \\ \times J_{2\rho_n} [2u] dt + k \exp \left[\frac{i\pi\eta}{2} - i\pi\rho_n + ikr + \frac{\pi\gamma}{2} \right] \int_0^\infty e^{-t} t^{-i\gamma} J_{2\rho_n+1} [2u] dt$$

$$(40b) \quad e^{i\eta_n G_n} = \left\{ (n+1-\sigma_n) + i(\gamma'-\gamma) \right\} \frac{1}{2} \frac{e^{ikr}}{r} e^{i\pi\eta/2} e^{-i\pi\sigma_n} \int_0^\infty e^{-t} t^{-i\gamma-1} J_{2\sigma_n} [2u] dt \\ - k \exp \left[ikr + \frac{\pi\gamma}{2} + \frac{i\pi\eta}{2} - i\pi\sigma_n \right] \int_0^\infty \frac{e^{-t} t^{-i\gamma}}{u} J_{2\sigma_n-1} (2u) dt.$$

In the non-relativistic limit ($\gamma' \rightarrow \gamma$, $\rho_n \rightarrow n$, etc.) the first term in both (40a) and (40b) approaches zero.

Substituting these expressions into (11a) one finds (exchanging the order of summation and integration),

$$(41) \quad \psi_3 = k e^{ikr+\pi\gamma/2} \int_0^\infty \frac{e^{-t} t^{-i\gamma}}{u} \sum_{n=0}^\infty \left\{ n J_{2\rho_n+1} (2u) e^{-i\pi\rho_n} - (n+1) J_{2\sigma_n-1} e^{-i\pi\sigma_n} \right\} \\ (-1)^{n_P} (\cos \theta) \\ + \frac{1}{2} \frac{e^{\pi\gamma/2 + ikr}}{r} \int_0^\infty e^{-t} t^{-i\gamma-1} \sum_{n=0}^\infty (-1)^{n_P} (\cos \theta) \left\{ \left[(n+1-\sigma_n) + i(\gamma'-\gamma) \right] \right. \\ \left. \times e^{-i\pi\sigma_n} J_{2\sigma_n} (n+1) + \left[(\rho_n - n) + i(\gamma'-\gamma) \right] n e^{-i\pi\rho_n} J_{2\rho_n} \right\} .$$

We next expand the Bessel functions of non-integral order about the integers to obtain

$$(42) \quad \psi_3 = k e^{i k r + \pi \gamma / 2} \int_0^{\infty} \frac{e^{-t} t^{-1 \gamma}}{u} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{m!} \left[n(\rho_n - n)^m + (n+1)(\sigma_n - n - 1)^m \right]$$

$$\frac{\partial^m}{\partial n^m} (J_{2n+1} e^{-i \pi n}) dt (-1)^n P_n(\cos \theta)$$

$$+ \frac{1}{2} \frac{e^{i k r + \pi \gamma / 2}}{r} \int_0^{\infty} e^{-t} t^{-1 \gamma - 1} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{m!} \left\{ \left[\rho_n - n \right]^m \left[(\rho_n - n) + i(\gamma' - \gamma) \right] \right.$$

$$\left. \frac{\partial^m}{\partial n^m} (J_{2n} e^{-i \pi n}) + \left[\sigma_n - n - 1 + i(\gamma' - \gamma) \right] \left[\sigma_n - n - 1 \right]^m \right.$$

$$\left. \frac{\partial^m}{\partial n^m} (J_{2n+2} e^{-i \pi n}) \right\} (-1)^n P_n(\cos \theta).$$

We shall now see that the relativistic correction terms cannot be obtained from the saddle point contribution. An inspection of the terms indicates that the corrections arise principally from the partial waves of low angular momentum or, in mathematical terms, from those terms in which $\sqrt{n^2 - \alpha^2}$ differs significantly from n . The saddle point previously obtained in dealing with the non-relativistic solutions corresponded, on the other hand, to large complex values of v , and, strictly speaking, the use of the method of steepest descent assumes that u and hence, v are large*.

* The use of the method as presented here is of doubtful validity inasmuch as an integration over all values of t from zero to infinity must be performed as indicated in (27) and $u = \sqrt{2ikr}$. The contribution from the interval 0 to $1/2ikr$ cannot be ignored. Asymptotic expansions of $\phi(a, c, x)$ for a, c and x all large would be useful in this connection as the integral representation would not have to be introduced. However, these are not known to the writer. [Those quoted in HTF, Vol. 1, p. 281-2 are not applicable.]

We shall consider only one term of the wave function, namely

$$(43) \quad h(r, \theta, \alpha, \gamma) \equiv k e^{ikr + \pi\gamma/2} \sum_{n=0}^{\infty} \int_0^{\infty} \frac{e^{-t} t^{-1\gamma}}{u} \left[n(\rho_n - n) + (n+1)(\sigma_n - n - 1) \right]$$

$$(-1)^{n_P} (\cos \theta) \frac{\partial}{\partial n} \left[e^{-i\pi n} J_{2n+1}(2u) \right] dt.$$

If an expansion of the radicals ρ_n and σ_n is made in powers of α^2 , the first term would be

$$(44) \quad - \frac{\alpha^2}{2} k e^{ikr + \pi\gamma/2} \left[2 \sum_{n=0}^{\infty} \int_0^{\infty} \frac{e^{-t} t^{-1\gamma}}{u} (-1)^{n_P} (\cos \theta) \frac{\partial}{\partial n} \left[e^{-i\pi n} J_{2n+1}(2u) \right] dt - \int_0^{\infty} \frac{e^{-t} t^{-1\gamma}}{u} \frac{\partial}{\partial n} \left[e^{-i\pi n} J_{2n+1}(2u) \right] \Big|_{n=0} dt \right]$$

Using the asymptotic expansion (32b) for the Bessel function, one has

$$(45) \quad \frac{\partial}{\partial v} (e^{-i\pi v} J_{2v+1}) \sim \left[-2i \chi - i\pi \right] e^{-i\pi v} J_{2v+1},$$

and repeating the procedure used above for the non-relativistic case, the method of steepest descent yields (considering α and γ to be independent)

$$(46) \quad h^{(1)}(r, \theta, 0, \gamma) = \frac{\partial h'(r, \theta, \alpha, \gamma)}{\partial \alpha^2} \Big|_{\alpha=0} \sim k \exp \left[ikr + \frac{\pi\gamma}{2} \right] l^{1/4} \cos \frac{\theta}{2} \int_0^{\infty} \frac{e^{-t} t^{-1\gamma}}{\sqrt{\pi u \sin \theta/2}} \times \left[(-i\theta - i\pi) \exp \left[2i u \sin \frac{\theta}{2} - \frac{i\pi}{4} \right] + (i\theta - i\pi) \exp \left[-2i u \sin \frac{\theta}{2} + \frac{i\pi}{4} \right] \right] dt.$$

The prime indicates that the last term in (44) has been dropped.

These integrals can be performed in terms of parabolic cylinder functions; one can then find the behavior for large kr . Using [38], [39]

$$(47) \quad \int_0^{\infty} e^{-t} t^{v'-1} \exp[-(2at)^{1/2}] dt = e^{a/2} 2^{1-v'} \Gamma(2v') D_{-2v'}(a^{1/2}),$$

$$\operatorname{Re} v' > 0,$$

$$(48a) \quad D_{-2v'}(a^{1/2}) \xrightarrow{a \rightarrow \infty} \frac{1}{a^{v'}} e^{-1/4a}, \quad -\frac{3\pi}{4} < \frac{1}{2} \arg a < -\frac{3\pi}{4},$$

$$(48b) \quad D_{-2v'}(a^{1/2}) \xrightarrow{a \rightarrow \infty} \frac{1}{a^{v'}} e^{-1/4a} - \frac{(2\pi)^{1/2}}{\Gamma(2v')} \frac{e^{-2i\pi v'}}{a^{1/2}}, \quad \frac{\pi}{4} < \frac{1}{2} \arg a < \frac{5\pi}{4},$$

one has:

$$(49) \quad h^{(1)}_{\nu}(r, \theta, 0, \gamma) \sim \frac{k \exp[ikr + \pi\gamma/2]}{4\sqrt{\pi} \cos \frac{\theta}{2} \sqrt[4]{2ikr \sin^2 \theta/2}} \\ \times \left\{ (-i\theta - i\pi) \frac{\exp[-ikr \sin^2 \theta/2] 2^{1/4 + i\gamma} \Gamma(3/2 - 2i\gamma)}{(4e^{-i\pi/2} kr \sin^2 \theta/2)^{3/4 - i\gamma}} \right. \\ + \frac{(i\theta - i\pi) 2^{1/4 + i\gamma} \exp[-ikr \sin^2 \theta/2] \Gamma(3/2 - 2i\gamma)}{(4e^{3\pi i/2} kr \sin^2 \theta/2)^{3/4 - i\gamma}} \\ \left. + \frac{(i\theta - i\pi) \exp[-2ikr \sin^2 \theta/2] (2\pi)^{1/2} 2^{1/4 + i\gamma}}{(4e^{3\pi i/2} kr \sin^2 \theta/2)^{1/2}} e^{2\pi(\gamma - \frac{3}{4}i)} \right\}$$

This is clearly incorrect; first, it is not of the form $\exp[ikr/r]$; secondly, it predicts an infinite cross section in the back direction ($\theta = \pi$).

In point of fact this term should yield the term

$$\pi\alpha\beta \sin \theta/2 (1 - \sin \theta/2)$$

in equation (C) and it will be shown later that

$$(50) \quad h^{(1)}(r, \theta, 0, 0) \xrightarrow{r \rightarrow \infty} \frac{\exp[ikr + i\gamma \ln 2kr]}{r} \frac{\pi\alpha^2}{4} \frac{1 - \sin \theta/2}{\sin \theta/2} .$$

For these reasons we will adopt a procedure equivalent to that of Mott and others and expand the phase shift in powers of α^2 and γ . Having done this we shall use the method of contour integration to sum the resulting series.

3. Calculation of cross section.

3.1 Expansion of the scattered field in powers of the fine structure constant.

For convenience each component of the wave is split into three parts. The expressions for the direct wave are:

$$(51a) \quad \psi_3^{(1)} = e^{ikr} e^{\pi\gamma/2} \int_0^\infty \frac{e^{-t} t^{-i\gamma}}{u} \sum_{k=0}^\infty (-1)^n P_n(\cos\theta) \\ \times \left[n \exp[-i\pi\sigma_n] J_{2\sigma_n+1} - (n+1) J_{2\sigma_n-1} \exp[-i\pi\sigma_n] \right] dt$$

$$(51b) \quad \psi_3^{(2)} = -\frac{(\gamma'-\gamma)}{2} \frac{e^{ikr}}{kr} e^{\pi\gamma/2} \int_0^\infty e^{-t} t^{-i\gamma-1} \sum_{n=0}^\infty (-1)^n P_n(\cos\theta) \\ \times \left[\exp[-i\pi\sigma_n] n J_{2\rho_n} + (n+1) J_{2\sigma_n} \exp[-i\pi\sigma_n] \right] dt$$

$$(51c) \quad \psi_j^{(3)} = \frac{i}{2} \frac{e^{ikr}}{kr} e^{\pi\gamma/2} \int_0^\infty e^{-t} t^{-1\gamma-1} \sum_{n=0}^\infty (-1)^n J_n(\cos\theta) \\ \times \left[n(\sigma_n - n) J_{2\sigma_n} \exp[-i\pi\sigma_n] - (n+1)(\sigma_n - (n+1)) J_{2\sigma_n} \exp[-i\pi\sigma_n] \right] dt$$

These equations are obtained directly from (41) but in doing so we have dropped a factor of k so as to later obtain an incident wave of absolute value unity. The results for ψ_4 can be written down by inspection of (11a), (11b) and (51). One sees that the changes to be made are as follows:

- a) replace $J_n(\cos\theta)$ by $J_n^{(1)}(\cos\theta)$ and multiply by $e^{i\phi}$;
- b) drop the factors of n and $n+1$, multiplying the Bessel functions;
- c) reverse the sign of the factor containing $J_{2\sigma_n}$ or $J_{2\sigma_n-1}$.

The use of three separate wave functions is equivalent to writing (13a) and (13b) as

$$(52a) \quad \exp[2i\eta_{-n-1}] = \frac{\Gamma(\sigma_n + 1 - i\gamma)}{\Gamma(\sigma_n + 1 + i\gamma)} \exp[i\pi(n - \sigma_n)] \left[1 + i \frac{\gamma - \gamma'}{\sigma_n - i\gamma} + \frac{n - \sigma_n}{\sigma_n - i\gamma} \right]$$

$$(52b) \quad \exp[2i\eta_n] = - \frac{\Gamma(\sigma_n + 1 - i\gamma)}{\Gamma(\sigma_n + 1 + i\gamma)} \exp[i\pi(n - \sigma_n)] \left[1 + i \frac{\gamma - \gamma'}{\sigma_n - i\gamma} + \frac{n + 1 - \sigma_n}{\sigma_n - i\gamma} \right].$$

The Bessel functions in equations (51a,b,c) and in the corresponding ones for ψ_4 are now expanded in a powers series about the integers and we obtain, for example [see equation 42]

$$\begin{aligned}
 (53) \quad \psi_3^{(1)} &= e^{ikr} e^{\pi\gamma/2} \int_0^\infty \frac{e^{-t} t^{-1\gamma}}{u} \sum_{n=0}^\infty \sum_{m=0}^\infty \frac{(-1)^n T_n(\cos\theta)}{m!} \\
 &\times \left\{ n \frac{\partial^m}{\partial v^m} (J_{2v+1} e^{-i\pi v}) [\rho_n - n]^m + (n+1) \frac{\partial^m}{\partial v^m} (J_{2v+1} e^{-i\pi v}) \right. \\
 &\times \left. [\rho_n - n - 1]^m \right\}.
 \end{aligned}$$

We consider that the factors such as $[\rho_n - n]$ are expanded in powers of α^2 . The t integration is carried out in all terms except the coefficient of the lowest power of α^2 in each of the three parts of ψ_3 and of ψ_4 . Taking the asymptotic form for large kr of the resulting expressions yields, with the exception of the six terms [the first three terms of ψ_3 and ψ_4] mentioned above, the form of the incident and scattered wave far from the nucleus. This procedure is of course entirely equivalent to a phase shift expansion and as such is really the same method as that employed by previous authors [5], [14] with this exception. The first terms in $\psi_3^{(3)}$ and $\psi_3^{(4)}$ contain sums of Bessel functions that are exactly summable. No further expansion of these terms (in powers of γ) is necessary. The first term of an expansion of these terms in powers of γ agrees with that of McKinley and Feshbach [14]. (Cf. their equation (6)ff. with our equation (56c)).

We shall concentrate first on these six terms involved and denote them in generally ψ' . One gets

$$\begin{aligned}
 (54a) \quad \psi_3'(1) &= e^{ikr} e^{\pi\gamma/2} \int_0^\infty \frac{e^{-t} t^{-i\gamma}}{u} \sum (2n+1) J_{2n+1}[2u] P_n(\cos\theta) dt \\
 &= e^{ikr} e^{\pi\gamma/2} \int_0^\infty e^{-t} t^{-i\gamma} J_0(2u \sin\theta/2) dt
 \end{aligned}$$

$$(54b) \quad \psi_3'(2) = -\frac{1}{2} (\gamma - \gamma') e^{\pi\gamma/2} \frac{e^{ikr}}{kr} \int_0^\infty \sum_{n=0}^\infty \left\{ n J_{2n} - (n+1) J_{2n+1} \right\}$$

$$\times P_n(\cos\theta) e^{-t} t^{-i\gamma-1} dt$$

$$= -\frac{1}{2} (\gamma - \gamma') e^{\pi\gamma/2} \frac{e^{ikr}}{kr} \sin\frac{\theta}{2} \int_0^\infty u J_1(2u \sin\theta/2) e^{-t} t^{-i\gamma-1} dt$$

$$\begin{aligned}
 (54c) \quad \psi_3'(3) &= \frac{i}{2kr} e^{\pi\gamma/2} \alpha^2 \int_0^\infty e^{-t} t^{-i\gamma-1} \left[\sum_{n=1}^\infty J_{2n} I_n(\cos\theta) + \sum_{n=0}^\infty J_{2n+1} P_n(\cos\theta) \right] dt \\
 &= -\frac{i}{2kr} e^{\pi\gamma/2} \alpha^2 \int_0^\infty e^{-t} t^{-i\gamma-1} \left[J_0(2u \sin\theta/2) - J_0(2u) \right] dt
 \end{aligned}$$

$$(54d) \quad \psi_4'(1) = 0$$

$$(54e) \quad \psi_4'(2) = \frac{1}{2} (\gamma - \gamma') e^{\pi\gamma/2} \frac{e^{ikr}}{kr} e^{i\phi} \int_0^\infty \sum_{n=0}^\infty (J_{2n} + J_{2n+1}) P_n^{(1)}(\cos\theta) e^{-t} t^{-i\gamma-1} dt$$

$$= -\frac{1}{2} (\gamma - \gamma') e^{\pi\gamma/2} \frac{e^{ikr}}{kr} e^{i\phi} \int_0^\infty u \cos\theta/2 J_1(2u \sin\theta/2) e^{-t} t^{-i\gamma-1} dt$$

$$= \cot\theta/2 e^{i\phi} \psi_3'(2)$$

$$\begin{aligned}
 (54f) \quad \psi_4^{(3)} &= \frac{1}{2kr} \exp[\pi \gamma/2] \alpha^2 \int_0^\infty e^{-t} t^{-i\gamma-1} \left[\sum_{n=1}^\infty \frac{J_{2n} P_n^{(1)}}{n} \right. \\
 &\quad \left. - \sum_{n=0}^\infty \frac{J_{2n+1}}{n+1} P_n^{(1)} \right] e^{-t} t^{-i\gamma-1} dt \\
 &= e^{i\phi} \frac{1}{2kr} \tan\theta/2 \exp[\pi \gamma/2] \alpha^2 \int_0^\infty e^{-t} t^{-i\gamma-1} [J_0(2u \sin\theta/2) - J_0(2u)] dt \\
 &= -\tan\theta/2 \psi_3^{(3)} e^{i\phi}
 \end{aligned}$$

In order to obtain the asymptotic behavior of these terms for large u we use [40].

$$(55) \quad \int_0^\infty e^{-t} t^{\alpha'} J_\beta [2(xt)^{1/2}] dt \xrightarrow{x \rightarrow \infty} e^{-x} x^{\alpha'} \exp[i\pi(\beta'/2 - \alpha)] + \frac{\Gamma(\beta'/2 + 1 + \alpha)}{\Gamma(\beta'/2 - \alpha)} (x)^{-\alpha-1}$$

and thus obtain, denoting the asymptotic form of ψ_j^i by u_j^i , $\ln \sin^2 \theta/2$ by λ and $\Gamma(1-i\gamma)/\Gamma(1+i\gamma)$ by $M(1)$

$$(56a) \quad u_3^{(1)} = \exp[ikz - i\gamma \ln 2kr \sin^2 \theta/2] + \frac{\gamma}{2k \sin^2 \theta/2} M(1) e^{i\gamma\lambda} \frac{\exp[ikr + i\gamma \ln 2kr]}{r}$$

$$(56b) \quad u_3^{(2)} = -M(1) \frac{\gamma - \gamma'}{2k} e^{i\gamma\lambda} \frac{\exp[ikr + i\gamma \ln 2kr]}{r}$$

$$(56c) \quad u_3'(3) = \frac{\alpha^2}{4k} M(1) \frac{e^{i\gamma\lambda} - 1}{\gamma} \frac{\exp[i\gamma \ln 2kr + ikr]}{r}$$

$$(56d) \quad u_4'(1) = 0$$

$$(56e) \quad u_4'(2) = \cot \theta/2 e^{i\phi} u_3'(2)$$

$$(56f) \quad u_4'(3) = -\tan \theta/2 e^{i\phi} u_3'(3)$$

The coefficients of $\frac{\exp[ikr + i\gamma \ln 2kr]}{r}$ in (56a,b,c,e,f) shall be denoted by $f_1', f_2', \alpha^2 f_3', g_2', \alpha^2 g_3'$ respectively. In applying (55) to obtain the behavior for large kr for $\psi_3'(3)$ and $\psi_4'(3)$, one should consider $J_0(2u \sin \theta/2) - J_0(2u)$

as $\lim_{\epsilon \rightarrow 0} J_\epsilon(2u \sin \theta/2) - J_\epsilon(2u)$ in order to satisfy the validity conditions specified by HTF.

In order to evaluate the remaining terms in the scattered waves, one applies (55) to (42), term by term, and in this manner obtains series of Legendre functions with coefficients involving

$\Gamma(n+1-i\gamma)/\Gamma(n+1+i\gamma)$. This function is expanded in an ascending power series in γ . For $v \sim c$, γ is approximately equal to α and therefore terms of order $\alpha^2 \gamma^2$, say, must be lumped with terms of order α^4 . If we denote the resulting series of Legendre functions occurring in u_3 as S_1 and those in u_4 as T_1 we have, for example

$$\begin{aligned}
 (57) \quad 2ku_3 = & \left\{ 2kf_1 + 2kf_2 + 2k\alpha^2 f_3 + \frac{\pi\alpha^2}{2} S_1 + \frac{\alpha^2 \gamma}{2} [2S_3 - 2i\pi S_2] \right. \\
 & + \frac{\alpha^2(\gamma-\gamma')}{2} [S_8 + i\pi S_9] - \frac{\alpha^2 \gamma^2}{2} [+ 2\pi S_4 + 4iS_5] \\
 & + \frac{\alpha^2(\gamma-\gamma')}{2} \gamma [2iS_{11} - 2iS_{10} - \pi S_6 + 2\pi S_{13} + 2iS_{12}] \\
 & \left. + \frac{\alpha^4}{8} [3\pi S_6 + i\pi^2 S_7 - 2iS_{11}] + \dots \right\} \frac{\exp[ikr + i\gamma \ln 2kr]}{r}
 \end{aligned}$$

The result for u_4 is analogous with the f 's replaced by the g 's and the S_i 's by the T_i 's. The T_i 's can be written down by inspection from the S_i 's by a method equivalent to that by which ψ_4 was obtained from ψ_3 . The series S_i and their sums as obtained by contour integration are tabulated in Table 1

The meaning of the symbols in Table 1 is as follows:

$$(58) \quad \psi_r(n+1) = \frac{d^r}{dn^r} \log \Gamma(n+1),$$

$$\mathcal{L}_2 = - \int_0^z \ln(1-\xi) d\xi / \xi, \quad \text{the dilogarithm of Euler,}$$

$$m = \frac{1 - \sin \theta/2}{1 + \sin \theta/2}.$$

3.2 The evaluation of the series.

As an example of the evaluation of the S_i 's by contour integration consider S_3 .

$$\begin{aligned}
 (60) \quad S_3 &= \sum_{1}^{\infty} \psi_2(n+1) P_n(\cos \theta) + \sum_{0}^{\infty} \psi_2(n+1) P_n(\cos \theta) \\
 &= \sum_{0}^{\infty} \psi_2(n+1) P_n(\cos \theta) - \psi_2(1)
 \end{aligned}$$

$$\begin{aligned}
 (61) \quad \sum \psi_2(n+1) P_n(\cos \theta) &= \frac{1}{2} \int_C \frac{P_v(-\cos \theta)}{\sin \pi v} \psi_2(v+1) dv \\
 &= -\frac{1}{2} \int_{-\infty}^{+\infty} \frac{P_{-1/2+i\tau}}{\cosh \pi \tau} \psi_2(1/2 + i\tau) d\tau
 \end{aligned}$$

In this last step we have distorted the path C , as indicated in Figure 2, so that the path of integration lies parallel to the imaginary v -axis after adding the circular arcs at infinity.

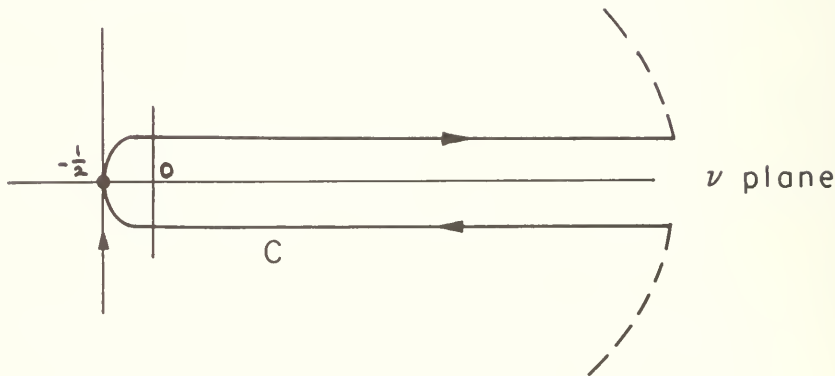


Figure 2

TABLE I

Part I - Sums appearing in cross-section.

$$(P_n = P_n(\cos \theta),$$

$$S_1 = \sum_{n=1}^{\infty} P_n + \sum_{n=0}^{\infty} P_n = \csc \theta/2 - 1$$

$$S_2 = \sum_{n=1}^{\infty} P_n \psi_1(n+1) + \sum_{n=0}^{\infty} P_n \psi_1(n+1) = \psi(1) [\csc \theta/2 - 1] - \csc \theta/2 [\ln(1 + \csc \theta/2) - \ln 4]$$

$$S_3 = \sum_{n=1}^{\infty} P_n \psi_2(n+1) + \sum_{n=0}^{\infty} P_n \psi_2(n+1) = \csc \theta/2 \left[\pi^2/4 - \mathcal{L}_2(m) + \mathcal{L}_2(-m) \right] - \pi^2/6$$

$$S_4 = \sum_{n=1}^{\infty} P_n \psi_1^2(n+1) + \sum_{n=0}^{\infty} P_n \psi_1^2(n+1) = \csc \theta/2 \left[\psi(1) + \ln(1 + \csc \theta/2) - \ln 4 \right]^2$$

$$+ \mathcal{L}_2(m) + \mathcal{L}_2(-m) - \pi^2/12 \Big] - \psi_1^2(1)$$

$$S_6 = \sum_{n=1}^{\infty} \frac{P_n}{n^2} + \sum_{n=0}^{\infty} \frac{P_n}{(n+1)^2} = 2 \mathcal{L}_2 \left(\frac{1}{1 + \sin \theta/2} \right) - 4 \mathcal{L}_2 \left(\frac{2 \sin \theta/2}{1 + \sin \theta/2} \right) - 4 \mathcal{L}_2 \left(\frac{1 + \sin \theta/2}{2} \right)$$

$$- 6 \mathcal{L}_2(1 - \sin \theta/2) - \ln^2(1 + \sin \theta/2) + 4 \ln 2 \ln(1 + \sin \theta/2) - 2 \ln^2 2$$

$$- 2 \ln \sin^2 \theta/2 \ln(1 + \sin \theta/2) + \frac{4\pi^2}{3} + S_8$$

$$S_8 = \sum_{n=1}^{\infty} \frac{P_n}{n^2} - \sum_{n=0}^{\infty} \frac{P_n}{(n+1)^2} = -\frac{1}{2} \frac{\partial^2}{\partial \nu^2} \frac{\pi \nu}{\sin \pi \nu} P_\nu(-\cos \theta) \Big|_{\nu=0} = \mathcal{L}_2(\cos^2 \theta/2) - \frac{\pi^2}{6}$$

$$S_9 = \sum_{n=1}^{\infty} \frac{P_n}{n} - \sum_{n=0}^{\infty} \frac{P_n}{(n+1)} = -2 \ln(1 + \sin \theta/2)$$

$$S_{13} = \sum_{n=1}^{\infty} \frac{P_n \psi_1(n+1)}{n} - \sum_{n=0}^{\infty} \frac{P_n \psi_1(n+1)}{n+1} = -4 \mathcal{L}_2 \left(\frac{2 \sin \theta/2}{1 + \sin \theta/2} \right) - 2 \mathcal{L}_2(1 - \sin \theta/2)$$

$$- \mathcal{L}_2(m) - \mathcal{L}_2(-m) - 2\psi(1) \ln(1 + \sin \theta/2) + \ln^4 \ln(1 + \sin \theta/2)$$

$$- \ln^2(1 + \sin \theta/2) + 2 \ln \left[\frac{2 \sin \theta/2}{1 + \sin \theta/2} \right] \ln \left[\frac{1 + \sin \theta/2}{(1 - \sin \theta/2)^2} \right] + \frac{7\pi^2}{12}$$

Part 2 - Sums not appearing in cross-section.

$$S_5 = \psi(1) \left\{ \csc \frac{\theta}{2} \left[\frac{\pi^2}{4} + \mathcal{L}_2(-m) - \mathcal{L}_2(m) \right] - \frac{\pi^2}{6} \right\} + 2 \int_0^1 \frac{\ln|y|}{(1-y)} \sqrt{\ln \left| \frac{2(\sqrt{})^2 (y-\cos\theta) [(y-\cos\theta)C+\sin\theta+\sqrt{}]}{(\sin\theta-\sqrt{})y\sin\theta [(y-\cos\theta)C+\sin\theta+\sqrt{}]} \right|} dy,$$

$$\sqrt{} = \sqrt{(y-\cos\theta)^2 + \sin^2\theta} \quad , \quad C = \tan(\frac{\theta}{2} - \frac{\pi}{4})$$

$$S_7 = \sum_1^{\infty} \frac{P_n}{n} + \sum_0^{\infty} \frac{P_n}{n+1} = - \frac{\partial}{\partial v} \frac{\pi v}{\sin \pi v} P_1(-\cos\theta) \Big|_{v=0} = - \ln \sin^2 \theta / 2$$

$$S_{10} = \sum_1^{\infty} \frac{\omega_{n+1} \psi_{n+1}}{n^2} - \sum_0^{\infty} \frac{P_{n+1} \psi_{n+1}}{(n+1)^2} = \mathcal{L}_2(\cos^2 \theta / 2) - \frac{\pi^2}{6} - \frac{\pi^2}{6} \ln(1+\sin\theta/2)^2 - \frac{1}{2} \psi_3(1)$$

$$- \int_0^1 \mathcal{L}_2(x) (1 + \frac{1}{x}) + \frac{\ln^2|x|}{2} \frac{dx}{\sqrt{(x-\cos\theta)^2 + \sin^2\theta}}$$

Part 2 - continued

$$S_{11} = \sum_1^{\infty} \frac{1}{n^3} + \sum_0^{\infty} \frac{P_n}{(n+1)^3} = -\frac{1}{3!} \frac{\partial^3}{\partial \nu^3} \frac{\pi \nu}{\sin \pi \nu} \left. P_{\nu}(-\cos \theta) \right|_{\nu=0} = \int_0^1 \frac{\ln |\nu| \ln |1-\nu \cos^2 \theta/2|}{\nu(1-\nu)} d\nu$$

$$S_{12} = \sum_1^{\infty} \frac{P_n \psi_2(n+1)}{n} - \sum_0^{\infty} \frac{P_n \psi_2(n+1)}{(n+1)} = -\psi_3(1) - \frac{\pi^2}{6} \ln^2 \sin \theta/2 - \frac{\pi^2}{6} \ln(1 + \csc \theta/2)$$

$$- \int_0^1 \frac{\frac{1}{x} \left[\frac{x^2}{6} - \mathcal{L}_2(1-x) \right] + \frac{\ln^2 |x|}{2} + \mathcal{L}_2(1-x)}{\sqrt{(x-\cos \theta)^2 + \sin^2 \theta}} dx$$

Part III - Sums appearing in μ_4 .

In general, if $S_i = \sum_1^{\infty} f(n) P_n(\cos\theta) \pm \sum_0^{\infty} g(n) P_n(\cos\theta)$,

$$\text{then } T_1 = \sum_1^{\infty} f\left(\frac{n}{2}\right) P_n(\cos\theta) \mp \sum \frac{g(n)}{n+1} P_n(\cos\theta)$$

$$T_1 = -\tan \theta/2 S_1$$

$$T_2 = -\tan \theta/2 S_2 + \csc\theta S_9$$

$$T_3 = -\tan \theta/2 S_3 - \csc\theta S_8$$

$$T_4 = -\tan \theta/2 S_4 - \csc\theta S_6 + 2\csc\theta S_{13}$$

$$T_5 = -\tan \theta/2 S_5 + \csc\theta(S_{12} - S_{10} + S_{11})$$

$$T_6 = -\tan \theta/2 S_6$$

$$T_7 = -\tan \theta/2 S_7$$

$$T_8 = \cotn \theta/2 S_8$$

$$T_9 = \cotn \theta/2 S_9$$

$$T_{10} = \cotn \theta/2 S_{10} - \csc \theta S_{11}$$

$$T_{11} = -\tan \theta/2 S_{11}$$

$$T_{12} = \cotn \theta/2 S_{12} + \csc \theta S_{11}$$

$$T_{13} = \cotn \theta/2 S_{13} - \csc\theta S_6$$

The behavior of the integrand on these circular arcs is dominated by

$$\frac{P_v(-\cos\theta)}{\sin \pi v} \xrightarrow{|\operatorname{Im} v| \rightarrow \infty} \exp\left[-\theta |\operatorname{Im} v|\right] \quad \text{for } 0 < \theta < \pi \quad \text{and thus the}$$

integration over the circular arcs yields a vanishing small contribution

to the integral. Use is made of the following integral representations: $[41], [42]$

$$(62a) \quad P_v(-x) = \sqrt{\frac{2}{\pi}} \frac{\Gamma(1/2)}{\Gamma(v+1)\Gamma(-v)} \int_0^\infty \frac{\cosh[(v+1/2)t] dt}{\sqrt{\cosh t - x}},$$

$\operatorname{Re}(v) < 0$, $\operatorname{Re}(v+1) > 0$, + x not on the real axis between 1 and ∞ ;

$$(62b) \quad \psi_1(z) = \psi_1(1) + \int_0^\infty \frac{e^{-t} - e^{-tz}}{1 - e^{-t}} dt, \quad \operatorname{Re}(z) > 0;$$

$$(62c) \quad \psi_2(z) = \int_0^\infty \frac{te^{-tz}}{1 - e^{-t}} dt, \quad \operatorname{Re}(z) > 0;$$

in evaluation of the sums.

Since

$$(63) \quad \int_0^\infty \frac{\cos t\tau dt}{\sqrt{\cosh t - \cos \theta}} = \frac{1}{2} \int_{-\infty}^{+\infty} \frac{e^{it\tau} dt}{\sqrt{\cosh t - \cos \theta}}$$

we can write the sum, using the integral representations as

$$(64) \sum_{n=0}^{\infty} \psi_2(n+1) P_n(\cos \theta) = \frac{\sqrt{2}}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^{\infty} \frac{\xi e^{-\xi/2} e^{-i\tau \xi} e^{i\tau} d\xi d\tau}{(1-e^{-\xi}) \sqrt{\cosh t - \cos \theta}} d\xi d\tau.$$

Interchanging the order of integration and applying the Fourier integral theorem, we have

$$\begin{aligned} (65) \sum_0^{\infty} \psi_2(n+1) P_n &= \frac{\sqrt{2}}{2} \int_0^{\infty} \frac{d\xi \xi e^{-\xi/2}}{\sqrt{\cosh \xi - \cos \theta} (1-e^{-\xi})} \\ &= \int_0^1 \frac{dx \ln |x|}{[(x-\cos \theta)^2 + \sin^2 \theta]^{1/2} (x-1)} \quad \left[\text{using } x = e^{-\xi} \right] \\ &= \frac{-\csc \theta/2}{2} \int_{\theta/2}^{\theta-\pi/2} \ln \left| \frac{\cos(v-\theta)}{\cos v} \right| \frac{dv}{\sin v - \theta/2} \cdot \\ &\quad \left[\text{using } \tan v = \frac{x-\cos \theta}{\sin \theta} \right]. \end{aligned}$$

Hence, by use of the further substitutions $u = v - \theta/2$, $t = \tan u/2$

$$(66) \quad 2 \sum \psi_2(n+1) P_n(\cos \theta) = + \csc \theta/2 \int_0^{\tan \frac{\pi-\theta}{4}} \ln \left| \frac{(t-c)(t-d)}{(t+c)(t+d)} \right| \frac{dt}{t}$$

where $c = \tan \theta/2 + \sec \theta/2$, $d = \tan \theta/2 - \sec \theta/2$.

Finally

$$(67) \quad S_3 = \csc \theta/2 \left[\frac{\pi^2}{4} - \mathcal{L}_2 \left(\frac{1-\sin\theta/2}{1+\sin\theta/2} \right) + \mathcal{L}_2 \left(-\frac{1-\sin\theta/2}{1+\sin\theta/2} \right) \right] - \frac{\pi^2}{6}.$$

For some further details see Appendix 1

An interesting example is

$$(68) \quad S_8 = \sum_{n=1}^{\infty} \frac{P_n(\cos\theta)}{n^2} - \sum_{n=0}^{\infty} \frac{P_n(\cos\theta)}{(n+1)^2}$$

$$= + \frac{1}{2} \int_C \frac{P_v(-\cos\theta)}{\sin\pi v} \cdot \frac{2v+1}{v^2(v+1)^2} dv - \frac{1}{2\pi} \int_{\Gamma} \frac{P_v(-\cos\theta)}{v^3} \frac{\pi v}{\sin\pi v} dv.$$

Γ is here a circular path about the origin of radius less than $1/2$, say, taken in a clockwise direction. When the integral over C is distorted to run parallel to the imaginary v axis, it will have the factor

$$\int_{-\infty}^{+\infty} \frac{\tau \cosh i\tau \, d\tau}{(\tau^2 + 1/4)} = 0.$$

Evaluating the residue at zero of the integral along Γ one has

$$(69) \quad S_8 = -\frac{1}{2} \frac{\partial^2}{\partial v^2} \left(P_v(-\cos\theta) \frac{\pi v}{\sin\pi v} \right) \Big|_{v=0} = \mathcal{L}_2(\cos^2\theta/2) - \frac{\pi^2}{6}.$$

3.3 The cross section.

Since the leading term in the scattered wave amplitude is proportional to α (for $\alpha \simeq v$), knowledge of the wave function to terms in α^4 permits the calculation of the differential cross section up to

those terms proportional to α^5 . However, we are actually interested in the ratio of this cross section to the Rutherford cross section,

$$(70) \quad \sigma_R(\theta) = \frac{r^2}{4k^2 \sin^4 \theta/2} = \frac{(Ze^2)^2}{4m^2 v^2} (1-\beta^2) \csc^4 \theta/2 \quad [\text{Relativistic}]$$

The ratio $\sigma(\theta)/\sigma_R$, commonly denoted by R , will contain terms proportional to α^{n-1} if the wave function and cross section are known to order α^n and α^{n+1} respectively. We shall indicate the order in α to which the wave function has been calculated by a Roman numeral subscript. Then

$$(71a) \quad R_I = 1 - \beta^2 \sin^2 \theta/2$$

$$(71b) \quad R_{II} - R_I = \pi \alpha \beta S_1 \sin^2 \theta/2 = \pi \alpha \beta \sin \theta/2 (1 - \sin \theta/2)$$

$$(71c) \quad R_{III} - R_{II} = \frac{\alpha^2 \lambda^2}{2} \sin^2 \theta/2 + \frac{\pi^2 \alpha^2 \beta^2}{4} S_1^2 \sin^4 \theta/2 \sec^2 \theta/2 \\ + \frac{\alpha^2 \beta^2}{4} \lambda^2 \sin^4 \theta/2 \sec^2 \theta/2 + \alpha^2 \sin^2 \theta/2 (2S_7 + \beta^2 S_8)$$

$$(71d) \quad R_{IV} - R_{III} = \frac{\pi \alpha \beta}{4} Q' \lambda S_1 \sec^2 \theta/2 \sin^4 \theta/2 - \frac{\pi \alpha^3}{2\beta} Q^2 S_1 \sin^2 \theta/2 \\ + \pi \frac{\alpha^3 \beta}{2} S_1 (2S_7 + S_8) \sec^2 \theta/2 \sin^4 \theta/2 \\ + \pi \frac{\alpha^3 \beta}{2} (S_9 - 2S_2) \lambda \sin^4 \theta/2 \sec^2 \theta/2 + \frac{\pi \alpha^3}{\beta} [2S_2 - \beta^2 S_9] \sin^2 \theta/2 \\ + 2\pi \alpha^3 \beta S_{13} \sin^2 \theta/2 - \frac{2\pi \alpha^3}{\beta} S_4 \sin^2 \theta/2 - \frac{\pi \alpha^3 \beta}{4} \sin^2 \theta/2 S_6.$$

Here $Q = 2\psi(1) - \lambda$, $Q' = 4\psi(1) - \lambda$, $\psi(1) = -E$ (the Euler-Mascheroni constant .5772) and again $\lambda = \ln \sin^2 \theta/2$. It should be noted that the series S_5, S_7, S_{10}, S_{11} , and S_{12} contained in the scattering amplitude are not present in the cross section, for when $u_3 u_3^*$ is calculated these series appear in terms of the form

$$(72) \quad \gamma i \alpha^4 S \left[M(1) e^{i\gamma\lambda} - M(1) e^{-i\gamma\lambda} \right] \approx 2\gamma^2 \alpha^4 S \left[(\lambda - 2\psi(1)) \right] + \dots$$

Since this calculation is exact in the limit $\alpha \rightarrow 0$, $\frac{\alpha}{\gamma} \approx 1$ consistency requires that such terms be dropped unless the wave function (cross section) is known to order α^5 (α^6).

We have calculated the cross section using these formulas (equations (71a-d)) for scattering by lead ($Z = 82$, $\alpha = .598$) at a bombarding energy of 10 Mev ($\beta = .9976$). The results are plotted in Figure 3 along with the exact results of Doggett and Spencer.

4. The general form of the coefficient of α^n .

In general we can write that

$$(73) \quad U(\theta, \alpha, \gamma) = 2ik u_3(\theta, \alpha, \beta) = \sum_{r=0}^{\infty} \sum_{S=0}^{\infty} \frac{\alpha^r \gamma^S}{r! S!} U_{r,S}(\theta, 0, 0)$$

when

$$(74) \quad U_{r,S}(\theta, 0, 0) = \left. \frac{\partial^{r+S} U}{\partial \alpha^r \partial \gamma^S}(\theta, \alpha, \gamma) \right|_{\gamma=0, \alpha=0}$$

With an increasing amount of analytic labor one can find the $U_{r,S}$ by expansion of the phase shifts as sums of the form:

RATIO OF RELATIVISTIC CROSS-SECTION
TO RUTHERFORD SCATTERING CROSS-SECTION

$z = 82$, energy = 10 mev

● Doggett & Spencer

▲ R_{IV}

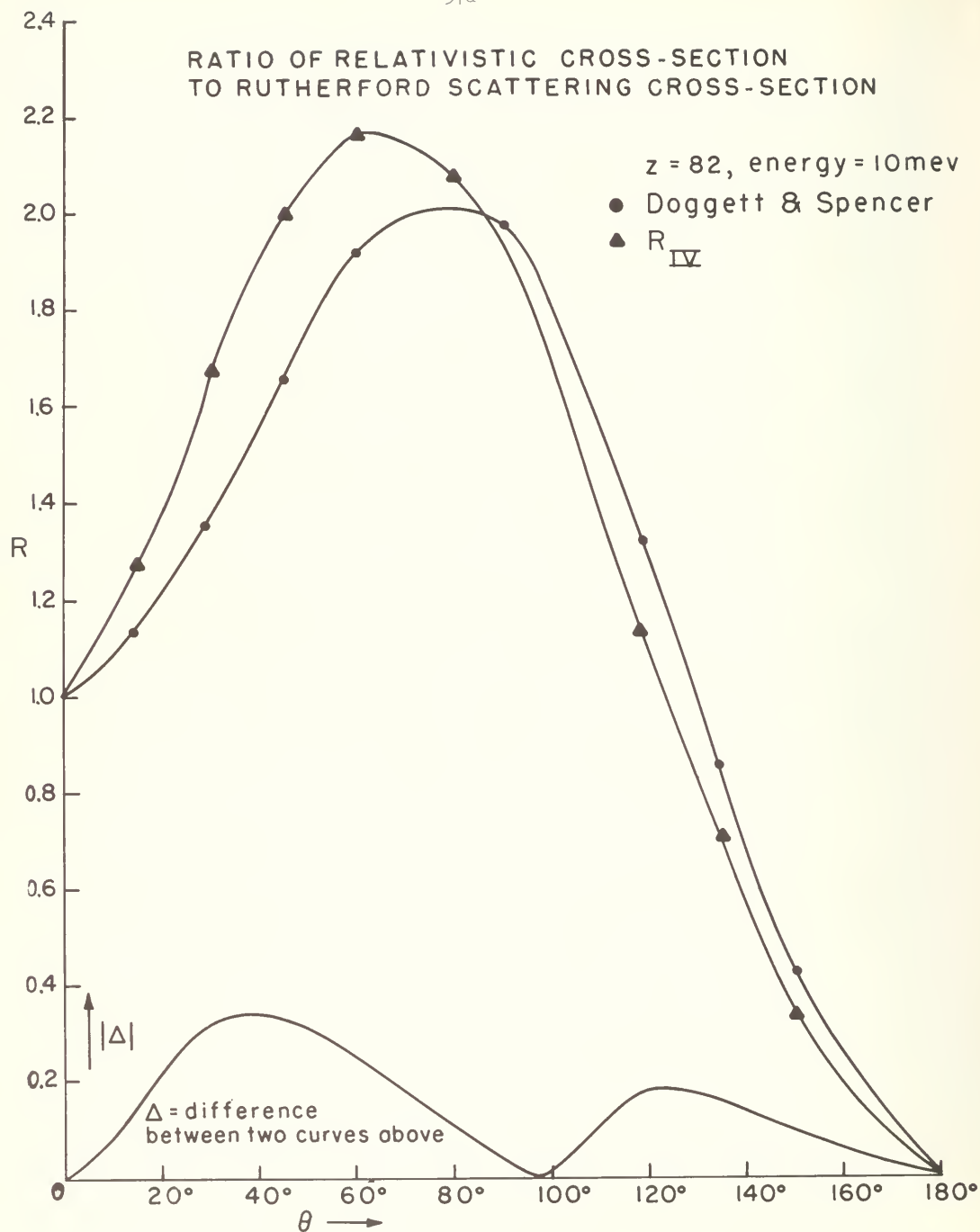


Figure 3

$$\sum_{n=1}^{\infty} f(n) (P_n(\cos \theta) \pm P_{n-1}(\cos \theta)) .$$

This, of course, was the starting point of the work described in the previous sections. By means of contour integration these sums were expressed in the form of integrals some of which can be evaluated in closed form. We shall now consider an alternative approach which bypasses the intermediate step, namely, expansion of the phase shift in powers of α and γ . The total scattering amplitude will first be expressed as a contour integral in the complex v -plane; integral representations will be used for certain functions and then derivatives with respect to α and γ will be taken. The result will be that the $U_{r,S}(\theta, 0, 0)$ can be expressed in terms of two dimensional real integrals. By a simple change in variables these integrals can be as integrals over a square in a two-dimensional space.

4.1 Non-relativistic scattering by an inverse cube law force.

Before considering the relativistic Coulomb problem itself we shall digress briefly to discuss a related problem. It is well known that the differential equation describing the motion of a relativistic classical particle moving in a Coulomb field differ from that of a non-relativistic particle in that the first contains an apparent force term proportional to $1/r^3$. It would appear reasonable to expect then that there will be mathematical similarities in the scattering amplitude for a particle obeying the non-relativistic Schrödinger equation moving in an inverse-cube-law force field and the scattering amplitude dealt with in this paper.

Formally one has the following differential equation:

$$(75) \quad -\frac{\hbar^2}{2m} \nabla^2 \chi - \frac{\gamma'}{r^2} \chi = \frac{\hbar^2}{2m} k^2 \chi,$$

with the boundary conditions:

$$(76) \quad \chi \xrightarrow{r \rightarrow \infty} e^{ikz} + h(\theta) \frac{e^{ikr}}{r}.$$

\$\chi\$ finite at the origin,

The solution is given by [43]

$$(77) \quad \chi = \sum (2n+1) P_n(\cos\theta) e^{-i\delta_n} j_{o_n}(kr)$$

where

$$\delta_n = -\frac{\pi}{2} \left[\sqrt{(n+\frac{1}{2})^2 - \eta^2} - (n+\frac{1}{2}) \right]$$

$$j_{o_n} = \sqrt{\frac{\pi}{2kr}} J_{o_n + 1/2} \text{ (spherical Bessel function)}$$

$$\eta^2 = 8\pi^2 m \gamma' / \hbar^2 < \frac{1}{4} \text{ (condition of regularity at origin)}$$

$$o_n = \sqrt{(n+\frac{1}{2})^2 - \eta^2} - \frac{1}{2}.$$

and

$$(78) \quad h(\theta, \eta) = \frac{1}{2ik} \sum_{n=0}^{\infty} (2n+1) P_n(\cos\theta) \left[e^{-2i\delta_n} - 1 \right]$$

$$(79) \quad H(\theta, \eta) = 2ikh(\theta, \eta) = \sum_{n=0}^{\infty} (2n+1) P_n(\cos\theta) \sum_{r=1}^{\infty} \frac{(i\pi)^r}{r!} \left[\sqrt{(n+\frac{1}{2})^2 - \eta^2} - (n+\frac{1}{2}) \right]^r$$

$$= \frac{i}{2} \int_D \frac{(2\nu+1) P_\nu(-\cos\theta)}{\sin \pi\nu} \sum_{r=1}^{\infty} \left[\sqrt{(\nu+\frac{1}{2})^2 - \eta^2} - \left(\nu+\frac{1}{2}\right) \right]^r \frac{(+i\pi)^r}{r!} d\nu$$

The contour D is shown in Figure 4 where the dashed portions indicate that the path lies on the second Riemann sheet of the functions $\sqrt{(v+1/2)^2 - \eta^2}$. The branch line extends from $v = -1/2 - \eta$ to $v = -1/2 + \eta$ and is indicated by a double line.

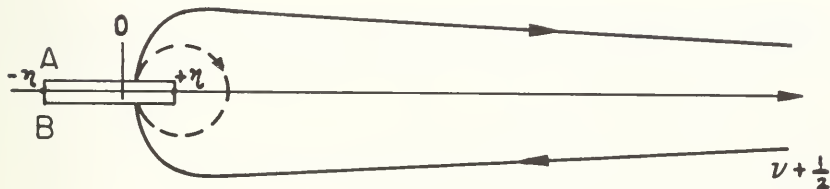


Figure 4

In the top sheet $\text{Im } \sqrt{(v+1/2)^2 - \eta^2} > 0$ at A and $\text{Im } \sqrt{(v+1/2)^2 - \eta^2} < 0$ at B. The portion of the path lying on the top Riemann sheet is now distorted so that it runs parallel to the imaginary v axis except for a small semi-circle centered about and lying to the right of the point $v = -1/2$. We have then

$$\begin{aligned}
 (80) \quad H(\theta, \eta) &= \frac{\sqrt{2} i}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{\tau e^{it\tau}}{\sqrt{\cosh t - \cos \theta}} \frac{(-\pi)^r}{r!} [K(\tau, \eta)]^r dt d\tau \\
 &\quad + \frac{i}{2} \int_{\Delta} \frac{(2v+1)P_v(-\cos \theta)}{\sin \pi v} \sum_{r=1}^{\infty} \frac{(i\pi)^r}{r!} \left[\sqrt{(v+1/2)^2 - \eta^2} - (v+1/2) \right]^r dv. \\
 \text{where } K(\tau, \eta) &= \begin{cases} \sqrt{\tau^2 + \eta^2} - \tau & \text{for } \tau > 0 \\ -\sqrt{\tau^2 + \eta^2} + (-\tau) & \text{for } \tau < 0. \end{cases}
 \end{aligned}$$

The contour Δ is the integral which lies in the bottom sheet. Upon inspection we see that a formal expansion of this integral in powers of η yields terms of the form

$$(81) \quad \eta^{2n} \oint_{\Delta} \frac{(2\nu+1)}{\sin \pi\nu} \frac{P_{\nu}(-\cos\theta)}{(\nu+1/2)^m} d\nu = 0$$

as no poles of the integrand are inclosed by the contour (for $\beta^2 < \frac{1}{4}$).

Note the discontinuous changes that occur for $\eta^2 = \frac{1}{4}$ and $\eta^2 > \frac{1}{4}$, values for which the scattering is undefined.

Consider now the function

$$g(\tau, \eta) = \sum_{r=1}^{\infty} \frac{a^r}{r!} \left[\sqrt{\tau^2 + \eta^2} - \tau \right]^r.$$

We desire, in general, the m^{th} derivative of this function with respect to η evaluated at $\eta = 0$. Using the integral representation^[44].

$$(82) \quad \sqrt{\tau^2 + \eta^2} - \tau = \eta \int_0^{\infty} \frac{e^{-\tau\lambda}}{\lambda} J_1(\eta\lambda) d\lambda$$

we find

$$(83a) \quad \frac{\partial^{2m}}{\partial \eta^{2m}} g(t, \eta) \Big|_{\eta=0} = 2m! \sum_{r=1}^m \frac{a^r}{r!} \frac{1}{\tau^{2m-r}} D(2m-r, r)$$

$$(83b) \quad \frac{\partial^{2m+1}}{\partial \eta^{2m+1}} g(t, \eta) \Big|_{\eta=0} = 0$$

where

$$(84) \quad D(2m-r, r) = \sum_{\substack{p_1+p_2+\dots+p_r=2m-r \\ p_i \text{ odd}}} C(2m-r; p_1, p_2, \dots, p_r),$$

$$(85) \quad C(2m-r, p_1 \dots p_r) = \frac{J_1^{(p_1)}(0) J_1^{(p_2)}(0) \dots J_1^{(p_r)}(0)}{p_1 p_2 \dots p_r},$$

and

$$(86) \quad J_1^{(p_i)}(0) = \frac{d^{p_i}}{dz^{p_i}} J_1(z) \Big|_{z=0}$$

Despite their seeming complexity the $D(2m-r, r)$ are simply rational fractions. For $\tau < 0$ we would find a similar result for the derivatives of $\left[-\sqrt{\tau^2 + \eta^2} + (-\tau) \right]$ except that τ in 83a would be replaced by $-(-\tau)$ which is just equal to τ . Thus

$$(87) \quad \frac{1}{m!} \frac{\partial^{2m} H(\theta, \eta)}{\partial \eta^{2m}} \Big|_{\eta=0} = \frac{\sqrt{2}}{2\pi} i \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \sum_{r=1}^m \frac{(-\pi)^r}{r!} \frac{1}{\tau^{2m-r-1}} \\ \updownarrow \\ \propto D(2m-r, r) \frac{e^{i\tau r}}{\sqrt{\cosh t - \cos \theta}} dt dr.$$

For $m > 1$, we have, using

$$(88) \quad \frac{1}{2\pi} \int_{\tau} \frac{e^{i\tau r}}{\tau^{2m-r-1}} = \begin{cases} -(2m-r-2)!(it)^{2m-r-2} & t > 0 \\ 0 & t < 0 \end{cases}$$

that \updownarrow

$$(89) \quad \frac{1}{m!} \frac{\partial^{2m}}{\partial \eta^{2m}} H(\theta, \eta) \Big|_{\eta=0} = -\sqrt{2} \sum_{r=1}^m (-\pi)^r \frac{(2m-r-2)!}{r!} D(2m-r, r) (i)^{2m-r-2} \\ \propto \int_0^{\infty} \frac{t^{2m-r-2}}{\sqrt{\cosh t - \cos \theta}} dt.$$

and for $m = 1$ that

$$(90) \quad \frac{1}{2!} \frac{\partial^2 H(\theta, \eta)}{\partial \eta^2} \Big|_{\eta=0} = \frac{-\pi i D(1,1)}{\csc \theta/2}$$

Since $D(1,1) = J_1^{(1)}(0) = 1/2$ the cross section to first order in η^2 would be given by

$$(91) \quad 4k^2 \sigma(\theta) = \frac{\pi^2 \eta^2}{4 \csc^2 \theta/2}$$

4.2 The general terms in Mott's expansion.

In treating the relativistic Coulomb scattering amplitude a similar procedure can be carried out; the exact form of the answer can be in several equivalent forms depending on the manner one uses to separate the phase shifts into distinct terms. We shall discuss the formulation used by Mott (cf. equations (14) and (15)) for two reasons: 1.) it can be more easily compared with previous work, and 2.) the notation is more compact.

The functions $F(\theta)$ and $G(\theta)$ were defined in equations (14a,b,c). These may be expressed as

$$(92a) \quad F(\theta) = \frac{i}{2} \sum_{n=0}^{\infty} (-1)^n n C_n \left[P_n(\cos \theta)_1 - P_{n-1}(\cos \theta) \right]$$

$$(92b) \quad G(\theta) = \frac{i}{2} \sum_{n=1}^{\infty} (-1)^n n^2 C_n \left[P_n(\cos \theta) + P_{n-1}(\cos \theta) \right]$$

Denoting by C_n^0 the function $-e^{-i\pi\nu} \frac{\Gamma(\nu-i\gamma)}{\Gamma(\nu+1+i\gamma)}$ and setting

$$(93) \quad D_n = C_n - C_n^0$$

one can rewrite (92) as

$$(94a) \quad F(\theta) = F_0 + F_1 = F_0 + \frac{1}{2} \sum (-1)^n n D_n [P_n(\cos\theta) - P_{n-1}(\cos\theta)]$$

$$(94b) \quad G(\theta) = G_0 + G_1 = G_0 + \frac{1}{2} \sum_{n=1}^{\infty} (-1)^n n^2 D_n [P_n(\cos\theta) - P_{n-1}(\cos\theta)]$$

where

$$(95) \quad F_0 = -\frac{i}{2k} \frac{\Gamma(1-i\gamma)}{\Gamma(1+i\gamma)} e^{i\gamma\lambda}$$

and

$$(96) \quad G_0 = i\gamma F_0 \cot^2 \theta/2 .$$

It should be noted here that Mott drops the sum $-\frac{1}{2ik} \sum_{n=0}^{\infty} (2n+1) P_n(\cos\theta)$

which is zero if θ differs from zero. Mott obtains the values of

F_0 and G_0 by physical considerations, namely by demanding that, in the

limit $c \rightarrow \infty$, $\alpha \rightarrow 0$, γ finite, the scattering amplitude reduces to

the non-relativistic value. Inasmuch as $C_n \xrightarrow{n \rightarrow \infty} \frac{-1}{n}$ and as thus

$n^2 C_n \xrightarrow{n \rightarrow \infty} -n$, this sum must be retained in a formal evaluation of G_0 .

This point requires further discussion, for similar considerations arise in more complicated fashion whenever expansion of the wave function are made by means of the Watson transformation in terms of

Legendre functions of non-integral order. The sum $\sum_{n=0}^{\infty} (2n+1) P_n(\cos\theta)$ represents symbolically the angular dependence of the outgoing wave portion of the incident wave. Thus one can find in some texts the expression [45]

$$(97) \quad e^{ikr \cos\theta} = \sum (2n+1) i^n j_n(kr) P_n(\cos\theta) \xrightarrow{r \rightarrow \infty} \sum \frac{2n+1}{2ikr} P_n(\cos\theta) \\ \times \left[e^{ikr} - (-1)^n e^{-ikr} \right].$$

This can be written as

$$(98) \quad e^{ikr \cos\theta} \xrightarrow{r \rightarrow \infty} \frac{1}{2ikr} \left[e^{ikr} \sum_0^{\infty} (2n+1) P_n(\cos\theta) P_n(\cos 0) \right. \\ \left. - e^{-ikr} \sum_0^{\infty} (2n+1) P_n(\cos\theta) P_n(\cos\pi) \right] = \frac{1}{ikr} e^{ikr} \delta(\cos\theta - \cos 0) \\ - e^{-ikr} \delta(\cos\theta - \cos \pi).$$

This is clearly incorrect; the basic error comes from using

$$(99) \quad j_n(kr) \xrightarrow{kr \rightarrow \infty} \frac{1}{kr} \cos(kr - (n+1)\pi/2).$$

However, no matter how large kr is made, there are values of n approximately equal to kr . It is for these values, which sum to $e^{ikr \cos\theta}$, that the asymptotic expression (99) is incorrect. In treating the scattering amplitude, however, such an expression can usually be used because the principal contribution to the difference between the total and incident waves comes from partial waves of value

$$n(n+1) \sim kb$$

where b is the wave number and b the radius of the region in which the potential energy is significantly comparable to the total energy.

In other words, in non-relativistic quantum scattering,

$$\frac{e^{ikr}}{2ikr} \sum (2n+1) P_n(\cos\theta) e^{2i\eta}$$

will not sum to the asymptotic form of the total wave but

$$\frac{e^{ikr}}{2ikr} \sum (2n+1) P_n(\cos\theta) [e^{2i\eta} - 1]$$

will give the outgoing scattered wave.

We shall now proceed to find the formal expression of the functions F and G in powers of α and $\beta = v/c$. For convenience we consider α and $\gamma = \alpha/\beta$ to be independent variables and the formal limit $\alpha \rightarrow$ not to imply $\gamma \rightarrow 0$. First we express P_n as [46]

$$(100) \quad P_n = \left(\cos\theta + \frac{\sin\theta}{n} \frac{d}{d\theta} \right) P_{n-1}$$

This is done in order that we can use the same integral representation employed previously in this paper despite a change in contour. Then

$$(101) \quad F = + \frac{1}{4} \int_{C'} \frac{e^{i\pi v}}{\sin \pi(v-1)} \left[(1-\cos\theta)v - \sin\theta \frac{\partial}{\partial \theta} \right] P_{v-1}(-\cos\theta) D(v) dv$$

where C' is the integral shown in Figure 5 and again

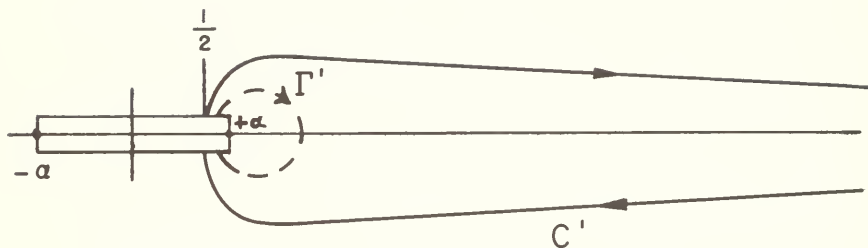


Figure 5

again the dotted contour Γ' indicates a path in the second Riemann sheet of the function $\sqrt{v^2 - a^2}$.

Distorting the contour C' so that it lies parallel to the imaginary v axis, we find, employing (83), that

$$\begin{aligned}
 (102) \quad \frac{1}{2m!} \frac{\partial^{2m} F_1}{\partial a^{2m}} \Big|_{a=0} &= \frac{\sqrt{2} i}{8\pi} \sum \frac{1}{r!} \frac{D(2m-r, r)}{\Gamma(1+2i\gamma)} \iint_{-\infty}^{+\infty} \\
 &\times \frac{\left[(1-\cos\theta)(1/2 + i\tau) - \sin\theta \frac{\partial}{\partial\theta} \right]}{(\tau - i/2)^{2m-r}} \frac{e^{i\tau r}}{\sqrt{\cosh t - \cos\theta}} \\
 &\times (\pi - i\xi)^r (1 - e^{-\xi})^{2i\gamma} e^{\xi(i\gamma - i\tau - 1/2)} d\xi dt d\tau
 \end{aligned}$$

and that

$$\begin{aligned}
 (103) \quad \frac{1}{2m!} \frac{1}{\ell!} \frac{\partial^{2m,\ell}}{\partial \alpha^{2m}} \frac{F_1}{\partial \gamma^\ell} \bigg|_{\alpha=0, \gamma=0} &= \frac{\sqrt{2} i}{8\pi} \sum \frac{2^\ell D(2m-r, r)}{r! s! (\ell-s)!} E(s) \\
 &\times \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^\infty \frac{[1 - \cos \theta] (1/2 + r i \pi) - \sin \theta \frac{\partial}{\partial \theta}}{(\tau - i/2)^{2m-r}} e^{i\tau(t-\xi) - \xi/2} \\
 &\times [\ln 2 \sinh \xi]^{-s} [\pi - i\xi]^r d\xi d\tau dt.
 \end{aligned}$$

Here

$$(104) \quad E(s) = \frac{d^s}{dx^s} \frac{1}{\Gamma(1+x)} \bigg|_{x=0}$$

and $E(0) = 1$, $E(1) = -\psi(1) = E$ (the Euler constant .577...). The use of the following recursion relation is useful to compute $E(s)$ for large values of s :

$$(105) \quad E(s+1) = \frac{d^s}{dx^s} - \frac{1}{\Gamma(1+x)} \psi(1+x) \bigg|_{x=0} = - \sum_{p=0}^n \binom{n}{p} E(s-p) \psi_{p+1}(1)$$

The $\psi_{p+1}(1)$'s are the polygamma functions.

In obtaining these last two results we have used [47]

$$(106) \quad \frac{\Gamma(v-i\gamma)}{\Gamma(v+1+i\gamma)} = \frac{1}{\Gamma(1+2i\gamma)} B(v-i\gamma, 1+2i\gamma) = \frac{1}{\Gamma(1+2i\gamma)} \int_0^\infty e^{-\xi(v-i\gamma)} (1-e^{-\xi})^{2i\gamma} d\xi$$

$$\operatorname{Re} v > 0$$

where B denotes the beta function.

We are now in a position to evaluate the integral over τ , i.e., to sum the partial waves. The integrals to be performed are of the form

$$(107) \quad \int_{-\infty}^{+\infty} \frac{e^{i\tau(t-\xi)}}{(\tau-i/2)^p} d\tau$$

and the result of this integration we shall denote symbolically as

$$(108) \quad 2\pi e^{-1/2(t-\xi)} i^p \delta_p(t-\xi)$$

where, if $\delta(t-\xi)$ is the Dirac delta function and p is positive:

$$(109) \quad \delta_p(t-\xi) = \int_{-\infty}^{t-\xi} \dots \int_{-\infty}^{u_2} \int_{-\infty}^{u_1} \delta(u_1) du_1 du_2 \dots du_p$$

p - fold

$$= \frac{1}{(p-1)!} (t-\xi)^{p-1} H(t-\xi) = \begin{cases} \frac{1}{(p-1)!} (t-\xi)^{p-1} & t > \xi \\ 0 & t < \xi \end{cases}$$

If p is negative, the corresponding derivative of the delta-function is indicated.

Finally then,

$$(110) \quad \left. \frac{\partial^{2m, \ell_F} 1}{\partial \alpha^{2m} \partial \gamma^\ell} \right|_{\alpha=0, \gamma=0} = \sqrt{2} i 2^{\ell-2} \sum_{r=1}^m \sum_{s=0}^e \frac{D(2m-r) E(s) i^{2m-r}}{r! s! (\ell-s)!}$$

$$\times \int_{-\infty}^{+\infty} \int_0^\infty \left[(1-\cos\theta) \delta_{2m-r-1}(t-\xi) - \delta_{2m-r}(t-\xi) \sin\theta \frac{\partial}{\partial \theta} \right] (\pi-i\xi)^r$$

$$\times \left[\ln 2 s \sinh \frac{r}{2} \right]^{-s} \frac{e^{-t/2}}{\sqrt{\cosh t - \cos \theta}} d\xi dt$$

and

$$\begin{aligned}
 (111) \quad & \frac{1}{2m!} \frac{\partial^{2m, \ell} G_1}{\partial \alpha^{2m} \partial \gamma^\ell} \bigg|_{\alpha=0, \gamma=0} = \sqrt{2} i 2^{\ell-2} \sum \frac{D(2m-r)E(s) i^{2m-r}}{r! s! (\ell-s)!} \\
 & \times \int_{-\infty}^{+\infty} \int_0^\infty \left[(1+\cos\theta) \delta_{2m-r-2}(t=\xi) + \delta_{2m-r-1}(t-\xi) \sin\theta \frac{\partial}{\partial \theta} \right] (\pi - i\xi)^r \\
 & \times \left[\ln 2 \sinh \frac{\xi}{2} \right]^{-s} \frac{e^{-t/2}}{\sqrt{\cosh t + \cos \theta}} d\xi dt .
 \end{aligned}$$

In general the form of the integrals will be:

$$\int_0^\infty \int_0^t \frac{e^{-t/2} (t-\xi)^{k_1} (i\pi-\xi)^{k_2} (\ln 2 \sinh \xi/2)^{k_3}}{(\cosh t - \cos \theta)^{1/2}} d\xi dt ;$$

(those involving the delta function and its derivative will be simpler).

The substitutions $y = e^{-\xi}$, $x = e^{-t}$ brings this into the form

$$(i\pi)^{k_4} \int_0^1 \int_x^1 \frac{\left[\ln \frac{y}{x} \right]^{k_1} \left[\ln y \right]^{k_2} \left[\ln \frac{1-y}{\sqrt{y}} \right]^{k_3}}{\sqrt{(x-\cos\theta)^2 + \sin^2 \theta}} \frac{dy}{y} dx .$$

As previously noted, the dilogarithm \mathcal{L}_2 is defined as

$$(112) \quad \mathcal{L}_2(z) = - \int_0^z \ln(1-\xi) \frac{d\xi}{\xi} .$$

A generalization, called the n-logarithm, is defined by [48]:

$$\mathcal{L}_n(z) = + \int_0^z \mathcal{L}_{n-1}(\xi) \frac{d\xi}{\xi} .$$

We may further generalize these as follows:

$$\mathcal{L}_{2,k}(z) = - \int_0^z [\ell n(1-\xi)]^k \frac{d\xi}{\xi} ;$$

$$\mathcal{L}_{n,k}(z) = \int_0^z \mathcal{L}_{n-1,k}(\xi) \frac{d\xi}{\xi} .$$

Integration by parts allows us to express $\mathcal{L}_{n,k}(z)$ as

$$\begin{aligned} \mathcal{L}_{n,k}(z) = & \ell n z \mathcal{L}_{n-1,k}(z) - \frac{\ell n^2 z}{2!} \mathcal{L}_{n-2,k} + \dots + (-1)^{n-1} \frac{\ell n^{n-2} z}{(n-2)!} \mathcal{L}_{2,k}(z) \\ & + \frac{(-1)^{n-1}}{(n-2)!} \int_0^z \frac{[\ell n \xi]^{n-2} [\ell n(1-\xi)]^k}{\xi} d\xi \end{aligned}$$

Finally then, the angular dependence of the correction terms to the scattered wave will be given by integrals of the form

$$(113) \quad \int_0^1 \frac{[\ell n x]^{m-1} [\ell n(1-x)]^m \mathcal{L}_{n,k}(1-x)}{\sqrt{(x-\cos\theta)^2 + \sin^2\theta}} dx .$$

5. Conclusions.

In this paper we have used the techniques of contour integration to obtain in closed form the differential cross section for relativistic Coulomb scattering up to the fifth order in the fine-structure-constant. The functional form of the relativistic corrections to the scattering amplitude corresponding to an arbitrary order of the fine structure constant were found in terms of two dimensional integrals involving elementary transcendental functions.

Appendix I

Evaluation of the Sums

In the evaluation of the sums listed in Table 1 integrals of the form:

$$\int_0^{\infty} \frac{e^{-t/2} f(t)}{\sqrt{\cosh t - \cos \theta}} dt, \quad f(t) \text{ real}, \quad (A')$$

arise. The substitution $x = e^{-t}$ casts the integrals into the form:

$$\int_0^1 \frac{f(-\ln x) dx}{\sqrt{(x - \cos \theta)^2 + \sin^2 \theta}} \quad (B')$$

Inasmuch as the integrals (A') are real one must take care that no imaginary terms appear in the final result. In particular the logarithm occurring in the integrals (B') must be considered to be $\ln|x|$. The dilogarithm and n-logarithm functions mentioned in the text require similar treatment. The following functional relations were used in simplifying the final results:

$$\mathcal{L}_2(x) + \mathcal{L}_2\left(\frac{1}{x}\right) = \frac{\pi^2}{3} - \frac{\ln^2|x|}{2};$$

$$\mathcal{L}_2(x) + \mathcal{L}_2(1-x) = \frac{\pi^2}{6} - \ln|x| \ln|1-x|.$$

These relations differ from those usually quoted for the reasons stated.

The derivatives of the Legendre functions with respect to order were calculated by differentiating the appropriate hypergeometric series term by term.

For example,

$$\begin{aligned}
 \left. \frac{\partial^2 P_v(-\cos\theta)}{\partial v^2} \right|_{v=0} &= \left. \frac{\partial^2}{\partial v^2} F(-v, v+1, 1, \frac{1+\cos\theta}{2}) \right|_{v=0} \\
 &= \frac{\partial^2}{\partial v^2} \left[1 - \frac{\sin\pi v}{\pi} \sum_{r=1}^{\infty} \frac{\Gamma(r+v+1)\Gamma(r-v)}{(r!)^2} (\cos^2\theta/2)^r \right] \Big|_{v=0} \\
 &= -2 \sum_{r=1}^{\infty} \frac{\Gamma(r+1)\Gamma(r)}{(r!)^2} [\Psi_1(r+1) - \Psi_1(r)] (\cos^2\theta/2)^r \\
 &= -2 \sum_{r=1}^{\infty} \frac{(\cos^2\theta/2)^r}{r^2} = -2 \mathcal{L}_2(\cos^2\theta/2)
 \end{aligned}$$

Here we have used the functional relation:

$$\Psi_1(r+1) = \Psi_1(r) + \frac{1}{r}.$$

The corresponding relationship for the polygamma functions follow by differentiation with respect to r .

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Research Reports and Publications

The following is a list of all research reports in the CX series.

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CX-1	S. Borowitz	The Schwinger Variational Method for Three-Body Collisions <u>Published</u> - Borowitz and Friedman, Phys. Rev., <u>89</u> , 441 (1953).	April, '52
CX-2	H. Moses	A Self-Consistent Calculation of the Dissociation of Oxygen in the Upper Atmosphere <u>Published</u> - Phys. Rev., <u>87</u> , 628 (1952).	April, '52
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CX-4	B. Friedman and E. Gerjuoy	Scattering Problems in Nonrelativistic Quantum Mechanics; Part I - One Particle in One Dimension	Dec., '52
CX-5	H. Moses	Exchange Scattering in a Three-Body Problem <u>Published</u> - Phys. Rev., <u>91</u> , (1953). Math. Rev., <u>16</u> , 1186 (1955).	Jan., '53
CX-6	H. Moses	Formulation of the Kohn-Hulthén Variational Principle in Terms of the Scattering Operator Formalism <u>Published</u> - Phys. Rev., <u>92</u> , 817 (1953). Math. Rev., <u>15</u> , 587 (1954).	April, '53
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(see CX-13)

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| CX-13 | H. Moses | The Scattering Operator in Quantum
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